Author Search

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=> FILE HCAPLUS
FILE 'HCAPLUS' ENTERED AT 12:27:02 ON 02 FEB 2009
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FILE COVERS 1907 - 2 Feb 2009  VOL 150 ISS 6
FILE LAST UPDATED: 1 Feb 2009  (20090201/ED)

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate
substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> D STAT QUE L32
L11             STR
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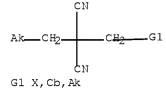

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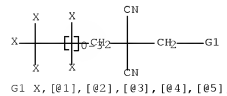

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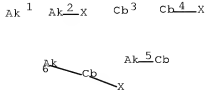

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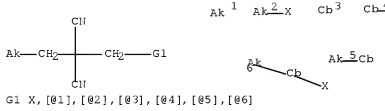


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L32           4 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  (L30 OR L31) AND (L28
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=> D IBIB ED ABS HITSTR L32 1-4

L32  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         2005:612241  HCAPLUS  Full-text
DOCUMENT NUMBER:          143:133096
TITLE:                    Preparation of nitrile compounds used in pest control
INVENTOR(S):              Gohira, Daisuke; Otaka, Ken
PATENT ASSIGNEE(S):       Sumitomo Chemical Company, Limited, Japan
SOURCE:                   PCT Int. Appl., 186 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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     WO 2005063694        A1    20050714    WO 2004-JP19692        20041222 <--
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
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			JP 2004-36230	A 20040213	
			JP 2004-283540	A 20040929	
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OTHER SOURCE(S): CASREACT 143:133096; MARPAT 143:133096

ED Entered STN: 15 Jul 2005

AB The present invention provides nitrile compds. RCH2C(CN)2CH2Q [R = C1-C4 fluoroalkyl, Q = halide, C1-C11 alkyl optionally substituted with halogen, C2-C6 alkenyl group optionally substituted with halogen, C2-C6 alkynyl optionally substituted with halogen, C3-C7 cycloalkyl optionally substituted with halogen or (C3-C7 cycloalkyl optionally substituted with halogen)C1-C4 alkyl] which have excellent effects against pests. For example, reacting Br(CH2)3Cl with F3C(CH2)2C(CN)2 gave F3C(CH2)2C(CN)2(CH2)3Cl. The compds. were used in many different formulations.

IT 913625-74-8 1044037-39-9

RL: PRPH (Prophetic)

(Preparation of nitrile compounds used in pest control)

RN 913625-74-8 HCAPLUS

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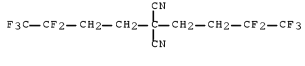

RN 1044037-39-9 HCAPLUS

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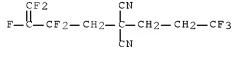

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858121-85-4P 913625-72-6P 913625-73-7P

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrile compds. as pesticides and their formulations)

RN 858120-92-0 HCAPLUS
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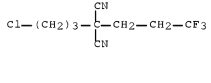

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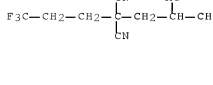

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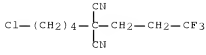
NAME)



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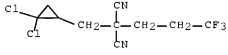

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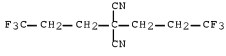

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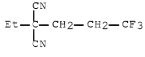

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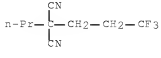

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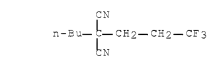

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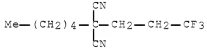

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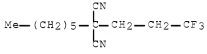

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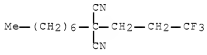

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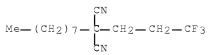

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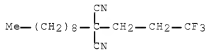

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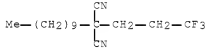

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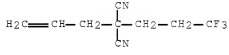

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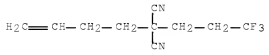

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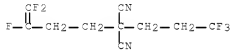

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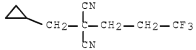

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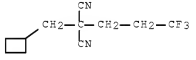

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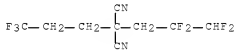

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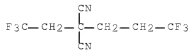

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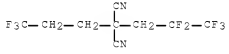

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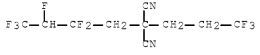
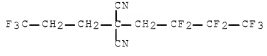
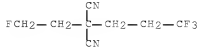


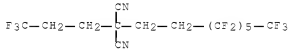
RN 858121-15-0 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,4-heptafluorobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



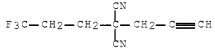
RN 858121-16-1 HCAPLUS
CN Propanedinitrile, 2-(2-fluoroethyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



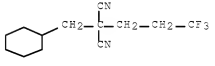
RN 858121-17-2 HCAPLUS
CN Propanedinitrile, 2-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



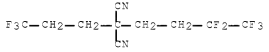
RN 858121-18-3 HCAPLUS
CN Propanedinitrile, 2-(2-propyn-1-yl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



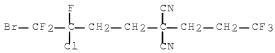
RN 858121-19-4 HCAPLUS
CN Propanedinitrile, 2-(cyclohexylmethyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



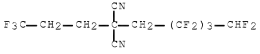
RN 858121-20-7 HCAPLUS
CN Propanedinitrile, 2-(3,3,4,4,4-pentafluorobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



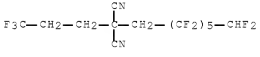
RN 858121-21-8 HCAPLUS
CN Propanedinitrile, 2-(4-bromo-3-chloro-3,4,4-trifluorobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



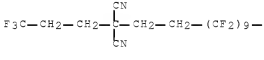
RN 858121-22-9 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



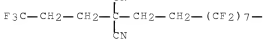
RN 858121-23-0 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



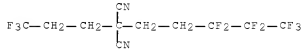
RN 858121-24-1 HCAPLUS
CN Propanedinitrile, 2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



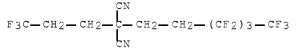
RN 858121-25-2 HCAPLUS
CN Propanedinitrile, 2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



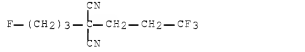
RN 858121-28-5 HCAPLUS
CN Propanedinitrile, 2-(3,3,4,4,5,5,5-heptafluoropentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



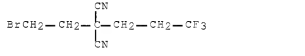
RN 858121-29-6 HCAPLUS
CN Propanedinitrile, 2-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



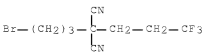
RN 858121-30-9 HCAPLUS
CN Propanedinitrile, 2-(3-fluoropropyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



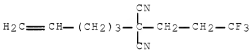
RN 858121-31-0 HCAPLUS
CN Propanedinitrile, 2-(2-bromoethyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



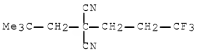
RN 858121-32-1 HCAPLUS
CN Propanedinitrile, 2-(3-bromopropyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



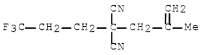
RN 858121-33-2 HCAPLUS
CN Propanedinitrile, 2-(4-penten-1-yl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



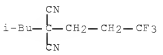
RN 858121-34-3 HCAPLUS
CN Propanedinitrile, 2-(2,2-dimethylpropyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



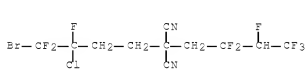
RN 858121-35-4 HCAPLUS
CN Propanedinitrile, 2-(2-methyl-2-propen-1-yl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



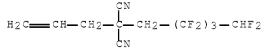
RN 858121-36-5 HCAPLUS
CN Propanedinitrile, 2-(2-methylpropyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



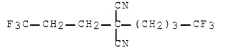
RN 858121-37-6 HCAPLUS
CN Propanedinitrile, 2-(4-bromo-3-chloro-3,4,4-trifluorobutyl)-2-(2,2,3,4,4,4-hexafluorobutyl)- (CA INDEX NAME)



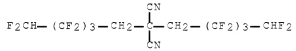
RN 858121-38-7 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(2-propen-1-yl)- (CA INDEX NAME)



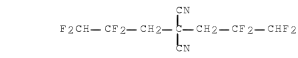
RN 858121-39-8 HCAPLUS
CN Propanedinitrile, 2-(4,4,4-trifluorobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



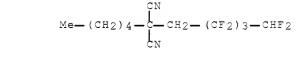
RN 858121-40-1 HCAPLUS
CN Propanedinitrile, 2,2-bis(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



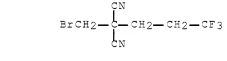
RN 858121-41-2 HCAPLUS
CN Propanedinitrile, 2,2-bis(2,2,3,3-tetrafluoropropyl)- (CA INDEX NAME)



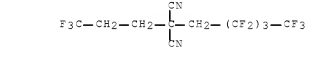
RN 858121-42-3 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-pentyl- (CA INDEX NAME)



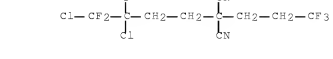
RN 858121-43-4 HCAPLUS
CN Propanedinitrile, 2-(bromomethyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



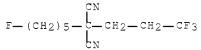
RN 858121-44-5 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5,5-nonafluoropentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



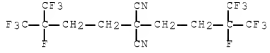
RN 858121-45-6 HCAPLUS
CN Propanedinitrile, 2-(3,4-dichloro-3,4,4-trifluorobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



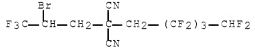
RN 858121-46-7 HCAPLUS
CN Propanedinitrile, 2-(5-fluoropentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



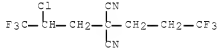
RN 858121-47-8 HCAPLUS
CN Propanedinitrile, 2,2-bis[3,4,4,4-tetrafluoro-3-(trifluoromethyl)butyl]- (CA INDEX NAME)



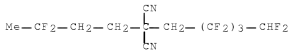
RN 858121-48-9 HCAPLUS
CN Propanedinitrile, 2-(2-bromo-3,3,3-trifluoropropyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



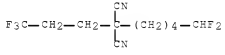
RN 858121-49-0 HCAPLUS
CN Propanedinitrile, 2-(2-chloro-3,3,3-trifluoropropyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



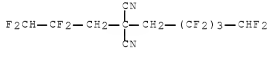
RN 858121-50-3 HCAPLUS
CN Propanedinitrile, 2-(3,3-difluorobutyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



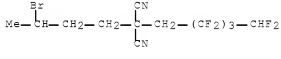
RN 858121-51-4 HCAPLUS
CN Propanedinitrile, 2-(5,5-difluoropentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



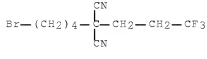
RN 858121-52-5 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(2,2,3,3-tetrafluoropropyl)- (CA INDEX NAME)



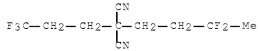
RN 858121-53-6 HCAPLUS
CN Propanedinitrile, 2-(3-bromobutyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



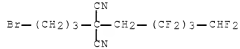
RN 858121-54-7 HCAPLUS
CN Propanedinitrile, 2-(4-bromobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



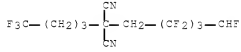
RN 858121-55-8 HCAPLUS
CN Propanedinitrile, 2-(3,3-difluorobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



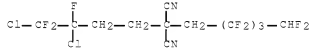
RN 858121-56-9 HCAPLUS
CN Propanedinitrile, 2-(3-bromopropyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



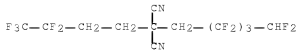
RN 858121-57-0 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(4,4,4-trifluorobutyl)- (CA INDEX NAME)



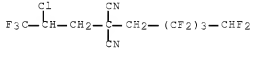
RN 858121-58-1 HCAPLUS
CN Propanedinitrile, 2-(3,4-dichloro-3,4,4-trifluorobutyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



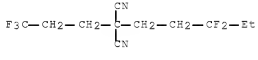
RN 858121-59-2 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(3,3,4,4,4-pentafluorobutyl)- (CA INDEX NAME)



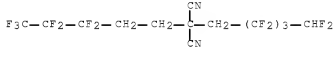
RN 858121-60-5 HCAPLUS
CN Propanedinitrile, 2-(2-chloro-3,3,3-trifluoropropyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



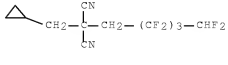
RN 858121-61-6 HCAPLUS
CN Propanedinitrile, 2-(3,3-difluoropentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



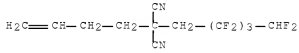
RN 858121-62-7 HCAPLUS
CN Propanedinitrile, 2-(3,3,4,4,5,5,5-heptafluoropentyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



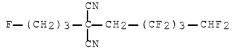
RN 858121-63-8 HCAPLUS
CN Propanedinitrile, 2-(cyclopropylmethyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



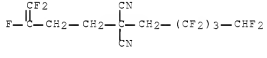
RN 858121-64-9 HCAPLUS
CN Propanedinitrile, 2-(3-buten-1-yl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)-
(CA INDEX NAME)



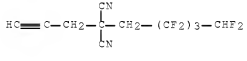
RN 858121-65-0 HCAPLUS
CN Propanedinitrile, 2-(3-fluoropropyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)-
(CA INDEX NAME)



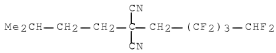
RN 858121-66-1 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(3,4,4-trifluoro-
3-buten-1-yl)- (CA INDEX NAME)



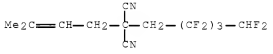
RN 858121-67-2 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(2-propyn-1-yl)-
(CA INDEX NAME)



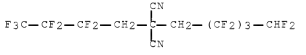
RN 858121-68-3 HCAPLUS
CN Propanedinitrile, 2-(3-methylbutyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)-
(CA INDEX NAME)



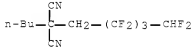
RN 858121-69-4 HCAPLUS
CN Propanedinitrile, 2-(3-methyl-2-buten-1-yl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



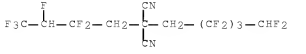
RN 858121-70-7 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,4-heptafluorobutyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



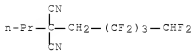
RN 858121-71-8 HCAPLUS
CN Propanedinitrile, 2-butyl-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



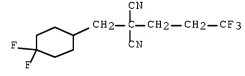
RN 858121-72-9 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,4,4,4-hexafluorobutyl)-2-(2,2,3,3,4,4,5,5-octafluoropentyl)- (CA INDEX NAME)



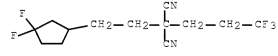
RN 858121-73-0 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-propyl- (CA INDEX NAME)



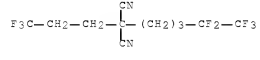
RN 858121-74-1 HCAPLUS
CN Propanedinitrile, 2-[(4,4-difluorocyclohexyl)methyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



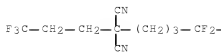
RN 858121-75-2 HCAPLUS
CN Propanedinitrile, 2-[2-(3,3-difluorocyclopentyl)ethyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



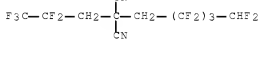
RN 858121-80-9 HCAPLUS
CN Propanedinitrile, 2-(4,4,5,5,5-pentafluoropentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



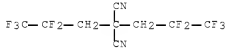
RN 858121-81-0 HCAPLUS
CN Propanedinitrile, 2-(4,4-difluoropentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



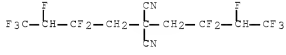
RN 858121-82-1 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(2,2,3,3,3-pentafluoropropyl)- (CA INDEX NAME)



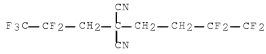
RN 858121-83-2 HCAPLUS
CN Propanedinitrile, 2,2-bis(2,2,3,3,3-pentafluoropropyl)- (CA INDEX NAME)



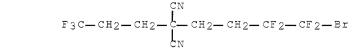
RN 858121-84-3 HCAPLUS
CN Propanedinitrile, 2,2-bis(2,2,3,4,4,4-hexafluorobutyl)- (CA INDEX NAME)



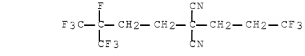
RN 858121-85-4 HCAPLUS
CN Propanedinitrile, 2-(3,3,4,4,5,5,5-heptafluoropentyl)-2-(2,2,3,3,3-pentafluoropropyl)- (CA INDEX NAME)



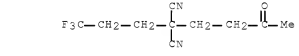
RN 913625-72-6 HCAPLUS
CN Propanedinitrile, 2-(4-bromo-3,3,4,4-tetrafluorobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



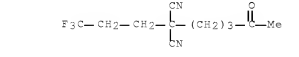
RN 913625-73-7 HCAPLUS
CN Propanedinitrile, 2-[3,4,4,4-tetrafluoro-3-(trifluoromethyl)butyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



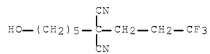
IT 676525-64-7P 676525-65-8P 858121-89-8P
858121-90-1P 858121-91-2P 858122-01-7P
913625-75-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrile compds. as pesticides and their formulations)
RN 676525-64-7 HCAPLUS
CN Propanedinitrile, 2-(3-oxobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



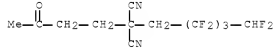
RN 676525-65-8 HCAPLUS
CN Propanedinitrile, 2-(4-oxopentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



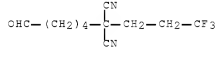
RN 858121-89-8 HCAPLUS
CN Propanedinitrile, 2-(5-hydroxypentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



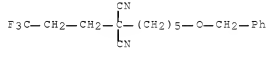
RN 858121-90-1 HCAPLUS
CN Propanedinitrile, 2-(2,2,3,3,4,4,5,5-octafluoropentyl)-2-(3-oxobutyl)- (CA INDEX NAME)



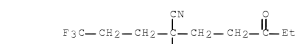
RN 858121-91-2 HCAPLUS
CN Propanedinitrile, 2-(5-oxopentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 858122-01-7 HCAPLUS
CN Propanedinitrile, 2-[5-(phenylmethoxy)pentyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 913625-75-9 HCAPLUS
CN Propanedinitrile, 2-(3-oxopentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:203802 HCAPLUS Full-text
DOCUMENT NUMBER: 140:235428
TITLE: Preparation of malononitrile compound and use thereof as pesticides
INVENTOR(S): Okada, Satoshi; Oohira, Daisuke; Otaka, Ken
PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004020399	A1	20040311	WO 2003-JP10726	20030826 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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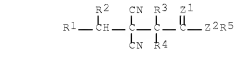
BR 2003013964	A	20050719	BR 2003-13964	20030826 <--
CN 1678571	A	20051005	CN 2003-820424	20030826 <--
CN 1315793	C	20070516		
JP 2004143148	A	20040520	JP 2003-208994	20030827 <--
US 20060004092	A1	20060105	US 2005-522764	20050201 <--
US 7439266	B2	20081021		
PRIORITY APPLN. INFO.:			JP 2002-250355 A	20020829 <--
			WO 2003-JP10726 W	20030826 <--

OTHER SOURCE(S): MARPAT 140:235428
ED Entered STN: 14 Mar 2004
GI

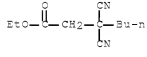


AB The present invention relates to a novel malononitrile compound represented by the formula (I): wherein, R1 represents C1 to C6 alkyl that may be substituted with halogen, C2 to C6 alkenyl that may be substituted with halogen, etc; R2 represents hydrogen atom or C1 to C6 alkyl that may be substituted with halogen; R3 represents hydrogen atom or C1 to C6 alkyl; R4 represents hydrogen atom or C1 to C6 alkyl; R5 represents C1 to C6 alkyl that may be substituted with halogen, C3 to C6 alkenyl that may be substituted with halogen, etc , or R4 and R5 may be combined at their terminal and represent ethylene that may be substituted with C1 to C3 alkyl or trimethylene that may be substituted with C1 to C3 alkyl; and Z1 and Z2, which are the same or different, represent oxygen atom or sulfur atom. Thus, 2-(tert-butoxycarbonylmethyl)-2-allylmalononitrile was prepared by reacting 2-allylmalonitrile with tert-Bu bromoacetate in DMF in the presence of sodium hydride. The malononitrile compound has an efficient pesticidal activity and can control effectively pests such as insect pests, acarine pests, nematode pests and the like.

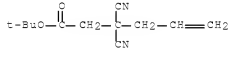
IT 436848-49-6P, 2-(Ethoxycarbonylmethyl)-2-butylmalononitrile
666738-57-4P, 2-(tert-Butoxycarbonylmethyl)-2-allylmalononitrile
666738-67-6P, 2-(Ethoxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile 666738-68-7P, 2-(Methoxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile
666738-69-8P, 2-(Butoxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile 666738-70-1P, 2-(Isopropoxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile
666738-71-2P, 2-(Isobutoxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile 666738-72-3P, 2-(sec-Butoxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile
666738-73-4P, 2-(Allyloxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile 666738-74-5P, 2-[(2-Butynyl)oxycarbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile
666738-75-6P, 2-(Hexyloxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile 666738-76-7P, 2-(Cyclohexyloxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile
666738-78-9P, 2-(tert-Butoxycarbonylmethyl)-2-(2-fluoroethyl)malononitrile 666738-80-3P, 2-(tert-Butoxycarbonylmethyl)-2-(3-chloropropyl)malononitrile
666738-81-4P, 2-(tert-Butoxycarbonylmethyl)-2-(3-chloro-2-methylpropyl)malononitrile 666738-82-5P, 2-(tert-Butoxycarbonylmethyl)-2-(4-chlorobutyl)malononitrile
666738-83-6P, 2-(tert-Butoxycarbonylmethyl)-2-(3-methyl-2-butenyl)malononitrile 666738-84-7P, 2-(tert-Butoxycarbonylmethyl)-2-butylmalononitrile 666738-85-8P, 2-(tert-Butoxycarbonylmethyl)-2-pentylmalononitrile 666738-86-9P , 2-(tert-Butoxycarbonylmethyl)-2-hexylmalononitrile 666738-87-0P , 2-(tert-Butoxycarbonylmethyl)-2-(3-methylbutyl)malononitrile
666738-90-5P, 2-(tert-Butoxycarbonylmethyl)-2-(cyclopropylmethyl)malononitrile 666738-91-6P, 2-(tert-Butoxycarbonylmethyl)-2-[(2,2-dichlorocyclopropyl)methyl]malononitrile 666738-92-7P, 2-(tert-Butoxycarbonylmethyl)-2-(2-butenyl)malononitrile
666738-93-8P, 2-(tert-Butoxycarbonylmethyl)-2-propylmalononitrile 666738-95-1P 666739-00-0P, 2-(tert-Butoxycarbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile
666739-01-1P, 2-[tert-Butoxy(thiocarbonyl)methyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-03-3P, 2-[(tert-Butylthio)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile
666739-04-4P, 2-(Methoxycarbonylmethyl)-2-butylmalononitrile
666739-05-5P, 2-(Butoxycarbonylmethyl)-2-butylmalononitrile

666739-06-6P, 2-(tert-Butoxycarbonylmethyl)-2-(4,4,4-trifluorobutyl)malononitrile 666739-07-7P, 2-[(2,2,2-Trifluoroethoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-08-8P, 2-[(2,2-Dimethylpropoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-09-9P, 2-[(2-Chloroethoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-10-2P, 2-[(2-Chloro-1-methylethoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-11-3P, 2-[(3-Chloropropoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-12-4P, 2-[(1,1-Dimethyl-2-propynyl)oxycarbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-13-5P, 2-((1-Ethyl-1-methyl-2-propynyloxycarbonyl)methyl)-2-(3,3,3-trifluoropropyl)malononitrile 666739-14-6P, 2-[(3-Methyl-3-methoxybutoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-15-7P, 2-[(1,1-Dimethyl-2-propenyl)oxycarbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-16-8P, 2-[(1,2-Dimethylpropoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-17-9P, 2-[(1-Cyano-1-methylethoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile 666739-27-1P, 2-([2,2,2-Trifluoro-1-(trifluoromethyl)ethoxy]carbonylmethyl)-2-(3,3,3-trifluoropropyl)malononitrile 666740-11-0P, 2-[(1,3-Dimethylbutoxy)carbonylmethyl]-2-(3,3,3-trifluoropropyl)malononitrile
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(production of malononitriles as pesticides)

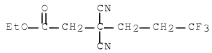
RN 436848-49-6 HCAPLUS
CN Heptanoic acid, 3,3-dicyano-, ethyl ester (CA INDEX NAME)



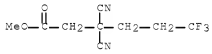
RN 666738-57-4 HCAPLUS
CN 5-Hexenoic acid, 3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



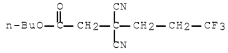
RN 666738-67-6 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, ethyl ester (CA INDEX NAME)



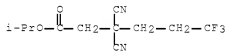
RN 666738-68-7 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, methyl ester (CA INDEX NAME)



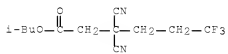
RN 666738-69-8 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, butyl ester (CA INDEX NAME)



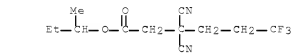
RN 666738-70-1 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 1-methylethyl ester (CA INDEX NAME)



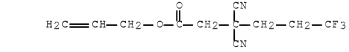
RN 666738-71-2 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 2-methylpropyl ester (CA INDEX NAME)



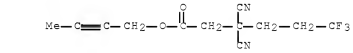
RN 666738-72-3 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 1-methylpropyl ester (CA INDEX NAME)



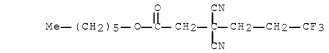
RN 666738-73-4 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 2-propen-1-yl ester (CA INDEX NAME)



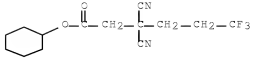
RN 666738-74-5 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 2-butyn-1-yl ester (CA INDEX NAME)



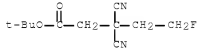
RN 666738-75-6 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, hexyl ester (CA INDEX NAME)



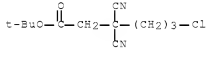
RN 666738-76-7 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, cyclohexyl ester (CA INDEX NAME)



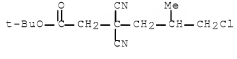
RN 666738-79-0 HCAPLUS
CN Pentanoic acid, 3,3-dicyano-5-fluoro-, 1,1-dimethylethyl ester (CA INDEX NAME)



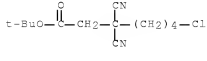
RN 666738-80-3 HCAPLUS
CN Hexanoic acid, 6-chloro-3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



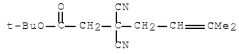
RN 666738-81-4 HCAPLUS
CN Hexanoic acid, 6-chloro-3,3-dicyano-5-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



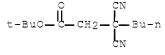
RN 666738-82-5 HCAPLUS
CN Heptanoic acid, 7-chloro-3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



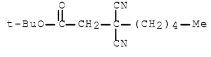
RN 666738-83-6 HCAPLUS
CN 5-Heptenoic acid, 3,3-dicyano-6-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



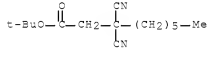
RN 666738-84-7 HCAPLUS
CN Heptanoic acid, 3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



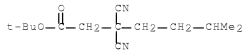
RN 666738-85-8 HCAPLUS
CN Octanoic acid, 3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



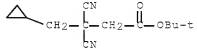
RN 666738-86-9 HCAPLUS
CN Nonanoic acid, 3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



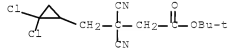
RN 666738-87-0 HCAPLUS
CN Heptanoic acid, 3,3-dicyano-6-methyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



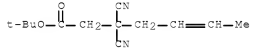
RN 666738-90-5 HCAPLUS
CN Cyclopropanebutanoic acid, β,β-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



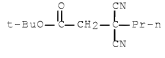
RN 666738-91-6 HCAPLUS
CN Cyclopropanebutanoic acid, 2,2-dichloro-β,β-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



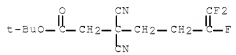
RN 666738-92-7 HCAPLUS
CN 5-Heptenoic acid, 3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



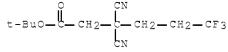
RN 666738-93-8 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-, 1,1-dimethylethyl ester (CA INDEX NAME)



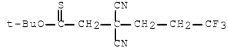
RN 666738-96-1 HCAPLUS
CN 6-Heptenoic acid, 3,3-dicyano-6,7,7-trifluoro-, 1,1-dimethylethyl ester (CA INDEX NAME)



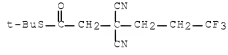
RN 666739-00-0 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 1,1-dimethylethyl ester (CA INDEX NAME)



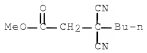
RN 666739-01-1 HCAPLUS
CN Hexanethioic acid, 3,3-dicyano-6,6,6-trifluoro-, O-(1,1-dimethylethyl) ester (CA INDEX NAME)



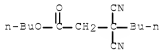
RN 666739-03-3 HCAPLUS
CN Hexanethioic acid, 3,3-dicyano-6,6,6-trifluoro-, S-(1,1-dimethylethyl) ester (CA INDEX NAME)



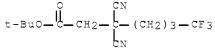
RN 666739-04-4 HCAPLUS
CN Heptanoic acid, 3,3-dicyano-, methyl ester (CA INDEX NAME)



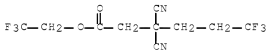
RN 666739-05-5 HCAPLUS
CN Heptanoic acid, 3,3-dicyano-, butyl ester (CA INDEX NAME)



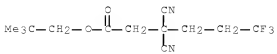
RN 666739-06-6 HCAPLUS
CN Heptanoic acid, 3,3-dicyano-7,7,7-trifluoro-, 1,1-dimethylethyl ester (CA INDEX NAME)



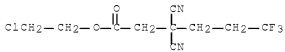
RN 666739-07-7 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 2,2,2-trifluoroethyl ester (CA INDEX NAME)



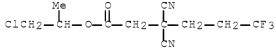
RN 666739-08-8 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 2,2-dimethylpropyl ester (CA INDEX NAME)



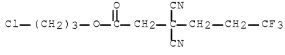
RN 666739-09-9 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 2-chloroethyl ester (CA INDEX NAME)



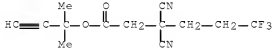
RN 666739-10-2 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 2-chloro-1-methylethyl ester (CA INDEX NAME)



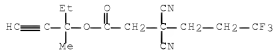
RN 666739-11-3 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 3-chloropropyl ester (CA INDEX NAME)



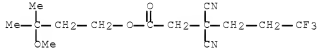
RN 666739-12-4 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 1,1-dimethyl-2-propyn-1-yl ester (CA INDEX NAME)



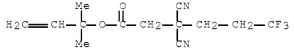
RN 666739-13-5 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 1-ethyl-1-methyl-2-propyn-1-yl ester (CA INDEX NAME)



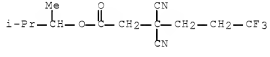
RN 666739-14-6 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 3-methoxy-3-methylbutyl ester (CA INDEX NAME)



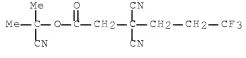
RN 666739-15-7 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 1,1-dimethyl-2-propen-1-yl ester (CA INDEX NAME)



RN 666739-16-8 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 1,2-dimethylpropyl ester (CA INDEX NAME)



RN 666739-17-9 HCAPLUS
CN Hexanoic acid, 3,3-dicyano-6,6,6-trifluoro-, 1-cyano-1-methylethyl ester (CA INDEX NAME)



RN 666739-27-1 HCAPLUS
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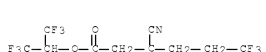

RN 666740-11-0 HCAPLUS
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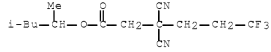

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:868901 HCAPLUS Full-text
DOCUMENT NUMBER: 137:352787
TITLE: Preparation of benzylmalononitriles as pesticides
INVENTOR(S): Otaka, Ken; Oohira, Daisuke; Okada, Satoshi
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002090320	A2	20021114	WO 2002-JP4449	20020508 <--
WO 2002090320	A3	20030220		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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JP 2003026510	A	20030129	JP 2002-120387	20020423	<--
TW 223979	B	20041121	TW 2002-91108311	20020423	<--
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CA 2446006	A1	20021114	CA 2002-2446006	20020508	<--
AU 2002255313	A1	20021118	AU 2002-255313	20020508	<--
AU 2002255313	B2	20070201			
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EP 1385817	B1	20081203			
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CN 101033200	A	20070912	CN 2007-10096610	20020508	<--
IN 2003CN01743	A	20060106	IN 2003-CN1743	20031104	<--
US 20040138065	A1	20040715	US 2003-477117	20031107	<--
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US 7402691	B2	20080722			
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PRIORITY APPLN. INFO.:

JP 2001-138331	A	20010509 <--
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WO 2002-JP4449	W	20020508 <--
IN 2003-CN1743	A3	20031104 <--
US 2003-477117	A3	20031107 <--

OTHER SOURCE(S): MARPAT 137:352787
ED Entered STN: 15 Nov 2002
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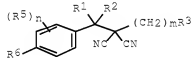

I

AB Title compds. [I; R1, R2 = (halo)alkyl, (halo)alkyloxy, (halo)alkenyl, (halo)alkynyl, H, cyano; R3 = haloalkyl, haloalkenyl, haloalkynyl; m = 1-3; R5 = halo, cyano, NO2, (halo)alkyl, (halo)alkenyl, (halo)alkynyl, (halo)alkylsulfonyl, (substituted) PhCH2O, PhO, PhS, etc.; n = 0-4; R6 = H, halo, cyano, NO2, (halo)alkyl, (halo)alkenyl, (halo)alkynyl, (halo)alkylsulfonyl, (halo)alkylcarbonyloxy, (substituted) PhCH2O, PhO, PhS, etc.; with provisos] were prepared Thus, 2-(4-chlorobenzyl)malononitrile in DMF was treated with NaH then with 2,3-dichloropropene under ice cooling followed by stirring at room temperature for 5 h to give 27% 2-(4-chlorobenzyl)-2-(2-chloro-2- propenyl)malononitrile. Numerous I at 500 ppm gave 100% kill of Musca domestica.

IT 474888-66-9P 474888-68-1P 474888-69-2P
474888-72-7P 474888-75-0P 474888-78-3P
474888-81-8P 474888-82-9P 474888-83-0P
474888-85-2P 474888-86-3P 474888-87-4P

474888-69-6P 474888-90-9P 474888-91-0P
474888-92-1P 474889-04-8P 474889-05-9P
474889-07-1P 474889-10-6P 474889-16-2P
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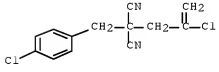
474889-35-5P 474889-36-6P 474889-40-2P
474889-44-6P 474889-45-7P 474889-46-8P
474889-47-9P 474889-48-0P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzylmalononitriles as pesticides)

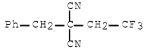
RN 474888-66-9 HCAPLUS

CN Propanedinitrile, 2-[(4-chlorophenyl)methyl]-2-(2-chloro-2-propen-1-yl)- (CA INDEX NAME)



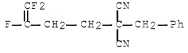
RN 474888-68-1 HCAPLUS

CN Propanedinitrile, 2-(phenylmethyl)-2-(2,2,2-trifluoroethyl)- (CA INDEX NAME)



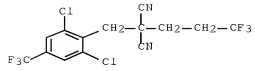
RN 474888-69-2 HCAPLUS

CN Propanedinitrile, 2-(phenylmethyl)-2-(3,4,4-trifluoro-3-buten-1-yl)- (CA INDEX NAME)



RN 474888-72-7 HCAPLUS

CN Propanedinitrile, 2-[[2,6-dichloro-4-(trifluoromethyl)phenyl]methyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 474888-75-0 HCAPLUS
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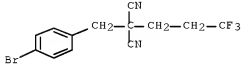
(CA INDEX NAME)



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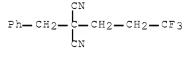
CN Propanedinitrile, 2-(phenylmethyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX
NAME)



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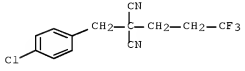

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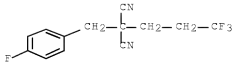
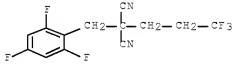
(CA INDEX NAME)



RN 474888-83-0 HCAPLUS
CN Propanedinitrile, 2-[(2,4,6-trifluorophenyl)methyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 474888-85-2 HCAPLUS
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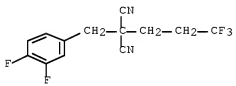

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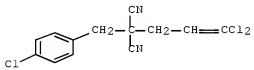

RN 474888-87-4 HCAPLUS
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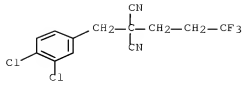
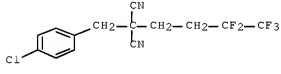
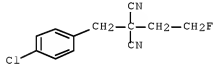


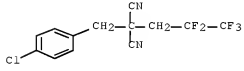
RN 474888-89-6 HCAPLUS
CN Propanedinitrile, 2-[(4-chlorophenyl)methyl]-2-(3,3,4,4,4-pentafluorobutyl)- (CA INDEX NAME)



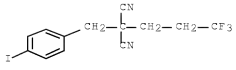
RN 474888-90-9 HCAPLUS
CN Propanedinitrile, 2-[(4-chlorophenyl)methyl]-2-(2-fluoroethyl)- (CA INDEX NAME)



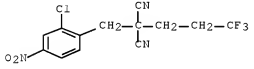
RN 474888-91-0 HCAPLUS
CN Propanedinitrile, 2-[(4-chlorophenyl)methyl]-2-(2,2,3,3,3-pentafluoropropyl)- (CA INDEX NAME)



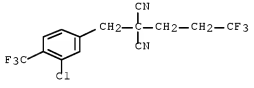
RN 474888-92-1 HCAPLUS
CN Propanedinitrile, 2-[(4-iodophenyl)methyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 474889-04-8 HCAPLUS
CN Propanedinitrile, 2-[(2-chloro-4-nitrophenyl)methyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 474889-05-9 HCAPLUS
CN Propanedinitrile, 2-[[3-chloro-4-(trifluoromethyl)phenyl]methyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 474889-07-1 HCAPLUS
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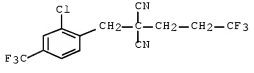

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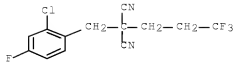
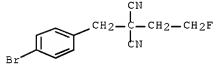
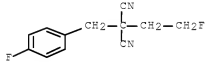


RN 474889-16-2 HCAPLUS
CN Propanedinitrile, 2-[(4-bromophenyl)methyl]-2-(2-fluoroethyl)- (CA INDEX NAME)

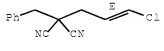


RN 474889-24-2 HCAPLUS
CN Propanedinitrile, 2-(2-fluoroethyl)-2-[(4-fluorophenyl)methyl]- (CA INDEX NAME)



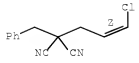
RN 474889-25-3 HCAPLUS
CN Propanedinitrile, 2-[(2E)-3-chloro-2-propen-1-yl]-2-(phenylmethyl)- (CA INDEX NAME)

Double bond geometry as shown.

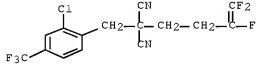


RN 474889-26-4 HCAPLUS
CN Propanedinitrile, 2-[(2Z)-3-chloro-2-propen-1-yl]-2-(phenylmethyl)- (CA INDEX NAME)

Double bond geometry as shown.



RN 474889-27-5 HCAPLUS
CN Propanedinitrile, 2-[[2-chloro-4-(trifluoromethyl)phenyl]methyl]-2-(3,4,4-trifluoro-3-buten-1-yl)- (CA INDEX NAME)



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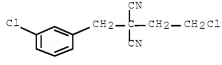

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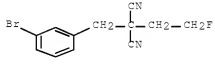
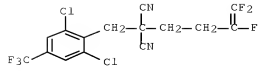


RN 474889-31-1 HCAPLUS
CN Propanedinitrile, 2-[[2,6-dichloro-4-(trifluoromethyl)phenyl]methyl]-2-(3,4,4-trifluoro-3-buten-1-yl)- (CA INDEX NAME)



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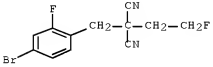
(CA INDEX NAME)



RN 474889-34-4 HCAPLUS
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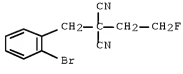
NAME)



RN 474889-35-5 HCAPLUS
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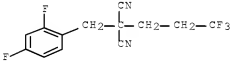
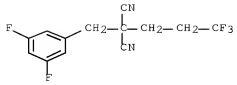
(CA INDEX NAME)



RN 474889-36-6 HCAPLUS
CN Propanedinitrile, 2-[(3,5-difluorophenyl)methyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



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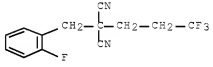
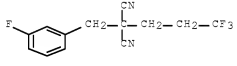
(CA INDEX NAME)



RN 474889-44-6 HCAPLUS
CN Propanedinitrile, 2-[(3-fluorophenyl)methyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



RN 474889-45-7 HCAPLUS
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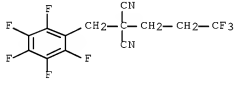
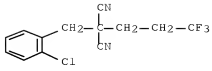
trifluoropropyl)- (CA INDEX NAME)



RN 474889-46-8 HCAPLUS
CN Propanedinitrile, 2-[(2-chlorophenyl)methyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



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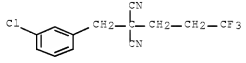
(CA INDEX NAME)



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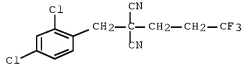
(CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:868658 HCAPLUS Full-text
DOCUMENT NUMBER: 137:369842
TITLE: Preparation of pesticidal benzylmalononitriles
INVENTOR(S): Otaka, Ken; Suzuki, Masaya; Oohira, Daisuke
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 109 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002089579	A1	20021114	WO 2002-JP4450	20020508 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT,				

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            LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT,
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     JP 2003026647          A     20030129     JP 2002-120386          20020423 <--
     JP 2003026510          A     20030129     JP 2002-120387          20020423 <--
     TW 223979              B     20041121     TW 2002-91108311        20020423 <--
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     AU 2002307746          A1    20021118     AU 2002-307746          20020508 <--
     EP 1385377             A1    20040204     EP 2002-769210          20020508 <--
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     CN 101033200           A     20070912     CN 2007-10096610        20020508 <--
     US 20040142821         A1    20040722     US 2003-476979          20031107 <--
PRIORITY APPLN. INFO.:                          JP 2001-138331      A   20010509 <--
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OTHER SOURCE(S):          MARPAT 137:369842
ED   Entered STN:  15 Nov 2002
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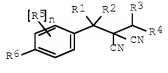

I

AB The title compds. [I; R1, R2 = (halo)alkyl, (halo)alkyloxy, (halo)alkenyl, (halo)alkynyl, H, CN; R3, R4 = C1-C10 alkyl, C2-C10 alkenyl, C2-C10 alkynyl, H; or R3 and R4 together form C2-C6 (halo)alkylene, C4-C6 (halo)alkenylene; R5 = halo, CN, NO2, (halo)alkyl, etc.; n = 0-4; R6 = H, halo, CN, NO2, (halo)alkyl, etc.; or R5 and R6 together form methylenedioxy; with the provisos that when R6 = H, then n = 1-4, and when n ≥ 2, then R5, R6 are different from each other], useful for controlling pests such as insect pests, acarine pests, and nematode pests, were prepared Thus, treating (4-chlorobenzyl)malononitrile (preparation given) with NaH in DMF followed by addition of allyl bromide afforded 54% 2-allyl-2-(4-chlorobenzyl)malononitrile which showed 100% control against Musca domestica, German cockroach and Cullex pipiens pallens at 500 ppm.

IT 475196-53-3P 475196-56-6P 475196-60-2P
475196-65-7P 475196-69-1P 475196-71-5P
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475197-15-0P 475197-19-4P 475197-21-8P
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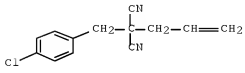
475197-70-7P 475197-72-9P 475197-76-3P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN

(Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pesticidal benzylmalononitriles)

RN 475196-53-3 HCAPLUS
CN Propanedinitrile, 2-[(4-chlorophenyl)methyl]-2-(2-propen-1-yl)- (CA INDEX NAME)



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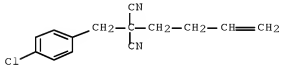

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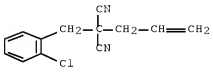
CN Propanedinitrile, 2-[(2-chlorophenyl)methyl]-2-(2-propen-1-yl)- (CA INDEX NAME)



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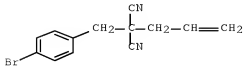
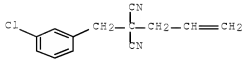


RN 475196-69-1 HCAPLUS
CN Propanedinitrile, 2-[(3-chlorophenyl)methyl]-2-(2-propen-1-yl)- (CA INDEX NAME)



RN 475196-71-5 HCAPLUS
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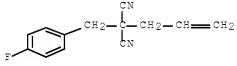

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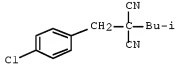

RN 475196-74-8 HCAPLUS
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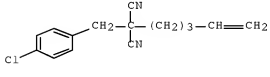

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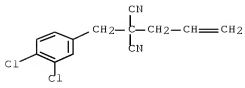

RN 475196-77-1 HCAPLUS
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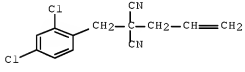

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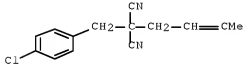

RN 475197-05-8 HCAPLUS
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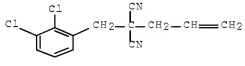

RN 475197-06-9 HCAPLUS
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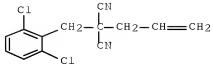

RN 475197-10-5 HCAPLUS
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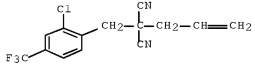

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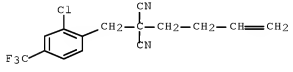

RN 475197-15-0 HCAPLUS
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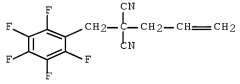
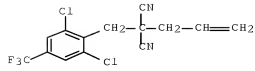
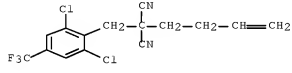


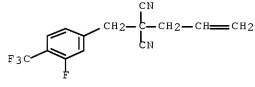
RN 475197-19-4 HCAPLUS
CN Propanedinitrile, 2-[[2,6-dichloro-4-(trifluoromethyl)phenyl]methyl]-2-(2-propen-1-yl)- (CA INDEX NAME)



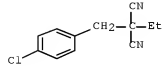
RN 475197-21-8 HCAPLUS
CN Propanedinitrile, 2-(3-buten-1-yl)-2-[[2,6-dichloro-4-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)



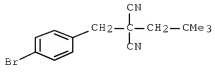
RN 475197-30-9 HCAPLUS
CN Propanedinitrile, 2-[[3-fluoro-4-(trifluoromethyl)phenyl]methyl]-2-(2-propen-1-yl)- (CA INDEX NAME)



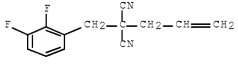
RN 475197-33-2 HCAPLUS
CN Propanedinitrile, 2-[(4-chlorophenyl)methyl]-2-ethyl- (CA INDEX NAME)



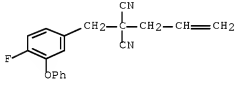
RN 475197-45-6 HCAPLUS
CN Propanedinitrile, 2-[(4-bromophenyl)methyl]-2-(2,2-dimethylpropyl)- (CA INDEX NAME)



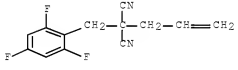
RN 475197-70-7 HCAPLUS
CN Propanedinitrile, 2-[(2,3-difluorophenyl)methyl]-2-(2-propen-1-yl)- (CA INDEX NAME)



RN 475197-72-9 HCAPLUS
CN Propanedinitrile, 2-[(4-fluoro-3-phenoxyphenyl)methyl]-2-(2-propen-1-yl)- (CA INDEX NAME)



RN 475197-76-3 HCAPLUS
CN Propanedinitrile, 2-(2-propen-1-yl)-2-[(2,4,6-trifluorophenyl)methyl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Structure Search

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L11             STR
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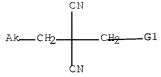

G1 X,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

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L20             STR
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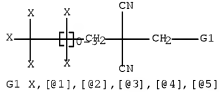

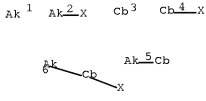

G1 X,[@1],[@2],[@3],[@4],[@5],[@6]

Structure attributes must be viewed using STN Express query preparation.

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L22           11 SEA FILE=REGISTRY SUB=L14 SSS FUL L20
L23            8 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L22
L29            2 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L23 AND (PRY<=2003 OR
                 AY<=2003 OR PY<=2003)


=> S L29 NOT L32
L33            0 L29 NOT L32

=> D STAT QUE L28
L11             STR
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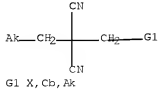

G1 X,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

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L24             STR
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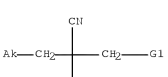


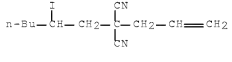
Gl X,[@1],[@2],[@3],[@4],[@5],[@6]

Structure attributes must be viewed using STN Express query preparation.
L26 493 SEA FILE=REGISTRY SUB=L14 SSS FUL L24
L27 154 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L26
L28 96 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L27 AND (PRY<=2003 OR AY<=2003 OR PY<=2003)

=> S L28 NOT L32,L29
L34 92 L28 NOT (L32 OR L29)

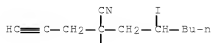
=> D IBIB ED ABS HITSTR L34 1-15; D IBIB ED ABS HITSTR L34 46-51; D IBIB ED ABS HITSTR 77-92 L34

L34 ANSWER 1 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1383584 HCAPLUS Full-text
DOCUMENT NUMBER: 149:555094
TITLE: Radical cyclization reactions
AUTHOR(S): Giese, B.; Kopping, B.; Gobel, T.; Dickhaut, J.; Thoma, G.; Kulicke, K. J.; Trach, F.
CORPORATE SOURCE: University Basel, Basel, Switz.
SOURCE: Organic Reactions (Hoboken, NJ, United States) (1996), 48, No pp. given
CODEN: ORHNBA
URL: http://www3.interscience.wiley.com/cgi-bin/mrwhome/107610747/HOME
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:555094
ED Entered STN: 19 Nov 2008
AB A review of the article Radical cyclization reactions.
IT 141314-52-5 141493-89-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(Radical Cyclization Reactions)
RN 141314-52-5 HCAPLUS
CN Propanedinitrile, 2-(2-iodohexyl)-2-(2-propen-1-yl)- (CA INDEX NAME)

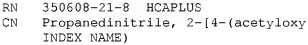


RN 141493-89-2 HCAPLUS

CN Propanedinitrile, 2-(2-iodohexyl)-2-(2-propyn-1-yl)- (CA INDEX NAME)



L34 ANSWER 2 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:994602 HCAPLUS Full-text
DOCUMENT NUMBER: 149:307001
TITLE: m-Trisulfonated Triphenylphosphine
AUTHOR(S): Michelet, Veronique; Savignac, Monique; Genet, Jean-Pierre
CORPORATE SOURCE: Fr.
SOURCE: e-EROS Encyclopedia of Reagents for Organic Synthesis (2001), No pp. given. John Wiley & Sons, Ltd.: Chichester, UK.
CODEN: 69KUHI
URL: http://www3.interscience.wiley.com/cgi-bin/mrwhome/104554785/HOME
DOCUMENT TYPE: Conference; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:307001
ED Entered STN: 19 Aug 2008
AB A review of the article m-Trisulfonated Triphenylphosphine.
IT 350608-21-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(m-Trisulfonated Triphenylphosphine)
RN 350608-21-8 HCAPLUS
CN Propanedinitrile, 2-[4-(acetyloxy)-2-buten-1-yl]-2-(2-propen-1-yl)- (CA INDEX NAME)



L34 ANSWER 3 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:268563 HCAPLUS Full-text
DOCUMENT NUMBER: 140:303319
TITLE: Preparation of malononitrile derivatives as pesticides and insecticides
INVENTOR(S): Takaoka, Daisuke; Otaka, Takeshi
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 89 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004099593	A	20040402	JP 2003-195617	20030711 <--
PRIORITY APPLN. INFO.:			JP 2002-208062 A	20020717 <--

OTHER SOURCE(S): MARPAT 140:303319

ED Entered STN: 02 Apr 2004

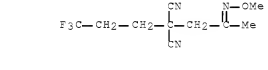
AB The title compds. R1ON:C(R2)(CR3R4)mC(CN)(CN)(CH2)nR5 [m = 0 - 3; n = 1 - 3; R1 = (halo-substituted) alkyl, etc.; R2 = (halo-substituted) alkyl, etc.; R3, R4 = H, (halo-substituted) alkyl, etc.; R5 = (halo-substituted) alkyl, etc.] are prepared Compds. of this invention at 500 ppm gave ≥ 90% kill of Musca domestica.

IT 676525-05-6P 676525-06-7P 676525-07-8P
676525-08-9P 676525-09-0P 676525-10-3P
676525-11-4P 676525-12-5P 676525-13-6P
676525-14-7P 676525-15-8P 676525-16-9P
676525-17-0P 676525-18-1P 676525-19-2P
676525-20-5P 676525-21-6P 676525-22-7P
676525-23-8P 676525-24-9P 676525-25-0P
676525-26-1P 676525-27-2P 676525-28-3P
676525-29-4P 676525-30-7P 676525-31-8P
676525-32-9P 676525-33-0P 676525-34-1P
676525-38-5P 676525-39-6P 676525-40-9P
676525-41-0P 676525-42-1P 676525-43-2P
676525-44-3P 676525-45-4P 676525-46-5P
676525-47-6P 676525-48-7P 676525-49-8P
676525-53-4P 676525-74-9P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of malononitrile derivs. as pesticides and insecticides)

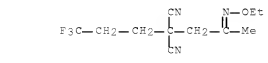
RN 676525-05-6 HCAPLUS

CN Propanedinitrile, 2-[2-(methoxyimino)propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



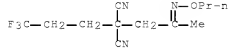
RN 676525-06-7 HCAPLUS

CN Propanedinitrile, 2-[2-(ethoxyimino)propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)

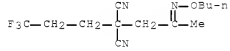


RN 676525-07-8 HCAPLUS

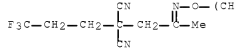
CN Propanedinitrile, 2-[2-(propoxyimino)propyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



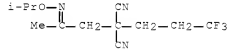
RN 676525-08-9 HCAPLUS
CN Propanedinitrile, 2-[2-(butoxyimino)propyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



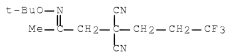
RN 676525-09-0 HCAPLUS
CN Propanedinitrile, 2-[2-[(pentyloxy)imino]propyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



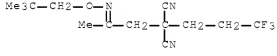
RN 676525-10-3 HCAPLUS
CN Propanedinitrile, 2-[2-[(1-methylethoxy)imino]propyl]-2-(3,3,3-
trifluoropropyl)- (CA INDEX NAME)



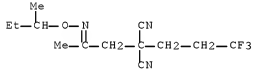
RN 676525-11-4 HCAPLUS
CN Propanedinitrile, 2-[2-[(1,1-dimethylethoxy)imino]propyl]-2-(3,3,3-
trifluoropropyl)- (CA INDEX NAME)



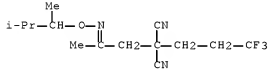
RN 676525-12-5 HCAPLUS
CN Propanedinitrile, 2-[2-[(2,2-dimethylpropoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



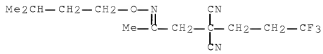
RN 676525-13-6 HCAPLUS
CN Propanedinitrile, 2-[2-[(1-methylpropoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



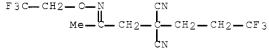
RN 676525-14-7 HCAPLUS
CN Propanedinitrile, 2-[2-[(1,2-dimethylpropoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



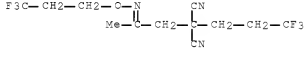
RN 676525-15-8 HCAPLUS
CN Propanedinitrile, 2-[2-[(3-methylbutoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



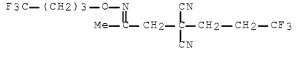
RN 676525-16-9 HCAPLUS
CN Propanedinitrile, 2-[2-[(2,2,2-trifluoroethoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



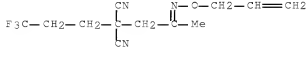
RN 676525-17-0 HCAPLUS
CN Propanedinitrile, 2-[2-[(3,3,3-trifluoropropoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



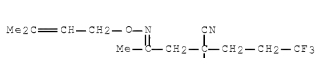
RN 676525-18-1 HCAPLUS
CN Propanedinitrile, 2-[2-[(4,4,4-trifluorobutoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



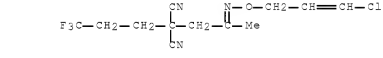
RN 676525-19-2 HCAPLUS
CN Propanedinitrile, 2-[2-[(2-propen-1-yloxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



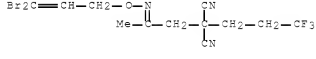
RN 676525-20-5 HCAPLUS
CN Propanedinitrile, 2-[2-[[(3-methyl-2-buten-1-yl)oxy]imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



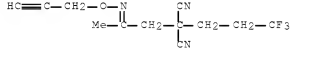
RN 676525-21-6 HCAPLUS
CN Propanedinitrile, 2-[2-[[(3-chloro-2-propen-1-yl)oxy]imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



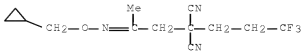
RN 676525-22-7 HCAPLUS
CN Propanedinitrile, 2-[2-[[(3,3-dibromo-2-propen-1-yl)oxy]imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



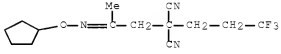
RN 676525-23-8 HCAPLUS
CN Propanedinitrile, 2-[2-[(2-propyn-1-yloxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



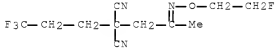
RN 676525-24-9 HCAPLUS
CN Propanedinitrile, 2-[2-[(cyclopropylmethoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



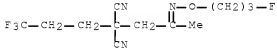
RN 676525-25-0 HCAPLUS
CN Propanedinitrile, 2-[2-[(cyclopentyloxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



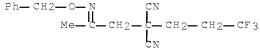
RN 676525-26-1 HCAPLUS
CN Propanedinitrile, 2-[2-[(2-fluoroethoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



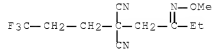
RN 676525-27-2 HCAPLUS
CN Propanedinitrile, 2-[2-[(3-fluoropropoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



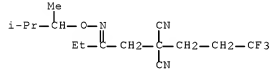
RN 676525-28-3 HCAPLUS
CN Propanedinitrile, 2-[2-[(phenylmethoxy)imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



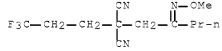
RN 676525-29-4 HCAPLUS
CN Propanedinitrile, 2-[2-(methoxyimino)butyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



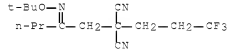
RN 676525-30-7 HCAPLUS
CN Propanedinitrile, 2-[2-[(1,2-dimethylpropoxy)imino]butyl]-2-(3,3,3-
trifluoropropyl)- (CA INDEX NAME)



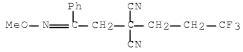
RN 676525-31-8 HCAPLUS
CN Propanedinitrile, 2-[2-(methoxyimino)pentyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



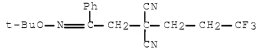
RN 676525-32-9 HCAPLUS
CN Propanedinitrile, 2-[2-[(1,1-dimethylethoxy)imino]pentyl]-2-(3,3,3-
trifluoropropyl)- (CA INDEX NAME)



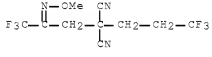
RN 676525-33-0 HCAPLUS
CN Propanedinitrile, 2-[2-(methoxyimino)-2-phenylethyl]-2-(3,3,3-
trifluoropropyl)- (CA INDEX NAME)



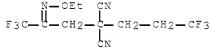
RN 676525-34-1 HCAPLUS
CN Propanedinitrile, 2-[2-[(1,1-dimethylethoxy)imino]-2-phenylethyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



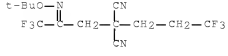
RN 676525-38-5 HCAPLUS
CN Propanedinitrile, 2-[3,3,3-trifluoro-2-(methoxyimino)propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



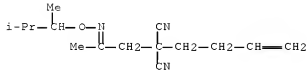
RN 676525-39-6 HCAPLUS
CN Propanedinitrile, 2-[2-(ethoxyimino)-3,3,3-trifluoropropyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



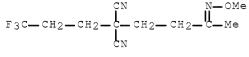
RN 676525-40-9 HCAPLUS
CN Propanedinitrile, 2-[2-[(1,1-dimethylethoxy)imino]-3,3,3-trifluoropropyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



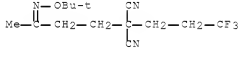
RN 676525-41-0 HCAPLUS
CN Propanedinitrile, 2-(3-buten-1-yl)-2-[2-[(1,2-dimethylpropoxy)imino]propyl]- (CA INDEX NAME)



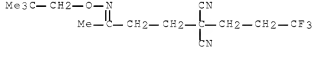
RN 676525-42-1 HCAPLUS
CN Propanedinitrile, 2-[3-(methoxyimino)butyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



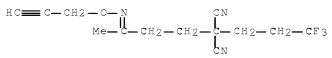
RN 676525-43-2 HCAPLUS
CN Propanedinitrile, 2-[3-[(1,1-dimethylethoxy)imino]butyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



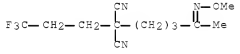
RN 676525-44-3 HCAPLUS
CN Propanedinitrile, 2-[3-[(2,2-dimethylpropoxy)imino]butyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



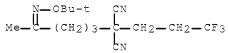
RN 676525-45-4 HCAPLUS
CN Propanedinitrile, 2-[3-[(2-propyn-1-yloxy)imino]butyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



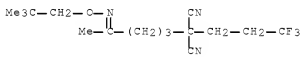
RN 676525-46-5 HCAPLUS
CN Propanedinitrile, 2-[4-(methoxyimino)pentyl]-2-(3,3,3-trifluoropropyl)-
(CA INDEX NAME)



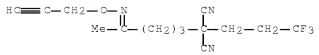
RN 676525-47-6 HCAPLUS
CN Propanedinitrile, 2-[4-[(1,1-dimethylethoxy)imino]pentyl]-2-(3,3,3-
trifluoropropyl)- (CA INDEX NAME)



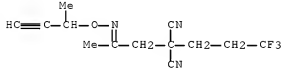
RN 676525-48-7 HCAPLUS
CN Propanedinitrile, 2-[4-[(2,2-dimethylpropoxy)imino]pentyl]-2-(3,3,3-
trifluoropropyl)- (CA INDEX NAME)



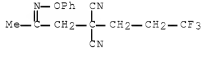
RN 676525-49-8 HCAPLUS
CN Propanedinitrile, 2-[4-[(2-propyn-1-yloxy)imino]pentyl]-2-(3,3,3-
trifluoropropyl)- (CA INDEX NAME)



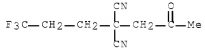
RN 676525-53-4 HCAPLUS
CN Propanedinitrile, 2-[2-[[(1-methyl-2-propyn-1-yl)oxy]imino]propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



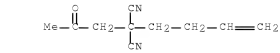
RN 676525-74-9 HCAPLUS
CN Propanedinitrile, 2-[2-(phenoxyimino)propyl]-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



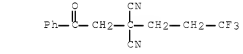
IT 676525-60-3P 676525-61-4P 676525-62-5P
676525-63-6P 676525-64-7P 676525-65-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of malononitrile derivs. as pesticides and insecticides)
RN 676525-60-3 HCAPLUS
CN Propanedinitrile, 2-(2-oxopropyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



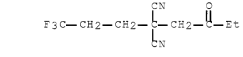
RN 676525-61-4 HCAPLUS
CN Propanedinitrile, 2-(3-buten-1-yl)-2-(2-oxopropyl)- (CA INDEX NAME)



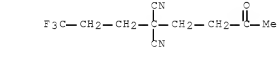
RN 676525-62-5 HCAPLUS
CN Propanedinitrile, 2-(2-oxo-2-phenylethyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



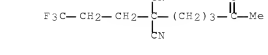
RN 676525-63-6 HCAPLUS
CN Propanedinitrile, 2-(2-oxobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



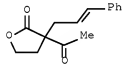
RN 676525-64-7 HCAPLUS
CN Propanedinitrile, 2-(3-oxobutyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)



RN 676525-65-8 HCAPLUS
CN Propanedinitrile, 2-(4-oxopentyl)-2-(3,3,3-trifluoropropyl)- (CA INDEX NAME)

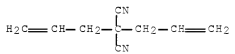


L34 ANSWER 4 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:729063 HCAPLUS Full-text
DOCUMENT NUMBER: 139:380992
TITLE: Triethylborane as an efficient promoter for palladium-catalyzed allylation of active methylene compounds with allyl alcohols
AUTHOR(S): Kimura, Masanari; Mukai, Ryutaro; Tanigawa, Naoko; Tanaka, Shuji; Tamaru, Yoshinao
CORPORATE SOURCE: Faculty of Engineering, Department of Applied Chemistry, Nagasaki University, 1-14 Bunkyo, Nagasaki, 852-8521, Japan
SOURCE: Tetrahedron (2003), 59(39), 7767-7777
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:380992
ED Entered STN: 17 Sep 2003
GI



I

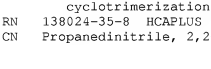
AB Allylation of a variety of active methylene compds. with allyl alcs. proceeds smoothly in the presence of catalytic amts. of Pd(OAc)2, Et3B, a phosphine ligand, and a base, to give allylated products, e.g. I, in good yields.
IT 90557-34-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium-catalyzed allylation of active methylene compds. with allylic alcs. in the presence of triethylborane)
RN 90557-34-9 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propen-1-yl- (CA INDEX NAME)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 5 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:726627 HCAPLUS Full-text
DOCUMENT NUMBER: 139:350530

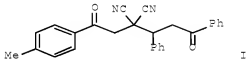
TITLE: Ruthenium(II)-Catalyzed Selective Intramolecular [2 + 2 + 2] Alkyne Cyclotrimerizations
AUTHOR(S): Yamamoto, Yoshihiko; Arakawa, Takayasu; Ogawa, Ryuji; Itoh, Kenji
CORPORATE SOURCE: Department of Applied Chemistry, Graduate School of Engineering, Nagoya University, Chikusa Nagoya, 464-8603, Japan
SOURCE: Journal of the American Chemical Society (2003), 125(40), 12143-12160
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:350530
ED Entered STN: 17 Sep 2003
AB In the presence of a catalytic amount of Cp*RuCl(cod), 1,6-diynes chemoselectively reacted with monoalkynes at ambient temperature to afford the desired bicyclic benzene derivs. in good yields. A wide variety of diynes and monoynes containing functional groups such as ester, ketone, nitrile, amine, alc., sulfide, etc. can be used for the present ruthenium catalysis. The most significant advantage of this protocol is that the cycloaddn. of unsym. 1,6-diynes with one internal alkyne moiety regioselectively gave rise to meta-substituted products with excellent regioselectivity. Completely intramol. alkyne cyclotrimerization was also accomplished using triyne substrates to obtain tricyclic aromatic compds. fused with 5-7-membered rings. A ruthenabicycle complex relevant to these cyclotrimerizations was synthesized from Cp*RuCl(cod) and O(CH2C.tplbond.CPh)2, and its structure was unambiguously determined by X-ray anal. The intermediacy of such a ruthenacycle was further confirmed by its reaction with acetylene, giving rise to the expected cycloadduct. The d. functional study on the cyclotrimerization mechanism elucidated that the cyclotrimerization proceeds via oxidative cyclization, producing a ruthenacycle intermediate and subsequent alkyne insertion initiated by the formal [2 + 2] cycloaddn. of the resultant ruthenacycle with an alkyne.
IT 138024-35-8, Dipropargylmalononitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(ruthenium(II)-catalyzed selective intramol. [2+2+2] alkyne cyclotrimerizations)
RN 138024-35-8 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propyn-1-yl- (CA INDEX NAME)



REFERENCE COUNT: 149 THERE ARE 149 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 6 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:657560 HCAPLUS Full-text
DOCUMENT NUMBER: 140:4821
TITLE: A facile synthesis of 1,6-diketones via a three-component Michael addition reaction
AUTHOR(S): Saikia, Anil; Chetia, Apurba; Bora, Utpal; Boruah,

Romesh C.
CORPORATE SOURCE: Medicinal Chemistry Division, Regional Research Laboratory, Jorhat, 785006, India
SOURCE: Synlett (2003), (10), 1506-1508
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:4821
ED Entered STN: 24 Aug 2003
GI

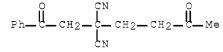


I

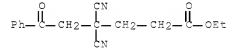
AB A convenient one-pot synthesis of 1,6-diketones, e.g., I, has been accomplished by a three-component Michael addition reaction of α-bromoketone, malononitrile, and α,β-unsatd. carbonyl compds.

IT 628338-98-7P 628339-01-5P 628339-02-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of diketones via three-component Michael reaction of bromoacetophenones with malononitrile and α,β-unsatd. ketones and esters)

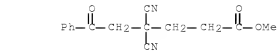
RN 628338-98-7 HCAPLUS
CN Propanedinitrile, 2-(3-oxobutyl)-2-(2-oxo-2-phenylethyl)- (CA INDEX NAME)



RN 628339-01-5 HCAPLUS
CN Benzenehexanoic acid, γ,γ-dicyano-ε-oxo-, ethyl ester (CA INDEX NAME)

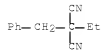


RN 628339-02-6 HCAPLUS
CN Benzenehexanoic acid, γ,γ-dicyano-ε-oxo-, methyl ester (CA INDEX NAME)

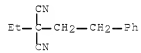


REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

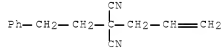
L34 ANSWER 7 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:580414 HCAPLUS Full-text
DOCUMENT NUMBER: 139:292031
TITLE: Enantioselective biotransformation of α,α-disubstituted dinitriles to the corresponding 2-cyanoacetamides using Rhodococcus sp. CGMCC 0497
AUTHOR(S): Wu, Zhong-Liu; Li, Zu-Yi
CORPORATE SOURCE: Shanghai Institute of Organic Chemistry, State Key Laboratory of Bioorganic & Natural Products Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Tetrahedron: Asymmetry (2003), 14(15), 2133-2142
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:292031
ED Entered STN: 30 Jul 2003
AB Nonracemic α,α-disubstituted-α-cyanoacetamides such as (S)-PhCH2C(Me)(CN)CONH2 (I) are prepared in 20-92% yields and in 2-99% ee by biotransformation of α,α-disubstituted-malononitriles in the presence of whole cells of Rhodococcus sp. CGMCC 0497. The α,α-disubstituted-malononitriles are prepared by alkylation of malononitrile with first a benzylic or phenethyl halide followed by alkylation with either Me iodide, Et bromide or allyl bromide. I is converted to either enantiomer of α-methylphenylalanine. Hofmann rearrangement of I followed by hydrolysis of the Me carbamate yields (S)-α-methylphenylalanine. Acid-mediated hydrolysis of the amide and esterification, peroxide-mediated hydrolysis of the nitrile, Hofmann rearrangement of the amide, and hydrolysis of the carbamate and carboxylic acid esters yields (R)-α-methylphenylalanine.
IT 21455-97-0P 606148-72-5P 606148-73-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of α,α-disubstituted malononitriles and their enantioselective biotransformation in the presence of Rhodococcus sp. CGMCC 0497 to yield nonracemic α,α-disubstituted-α-cyanoacetonitriles)
RN 21455-97-0 HCAPLUS
CN 1,1-Propanedinitrile, 1-(phenylmethyl)- (CA INDEX NAME)



RN 606148-72-5 HCAPLUS
CN Propanedinitrile, 2-ethyl-2-(2-phenylethyl)- (CA INDEX NAME)

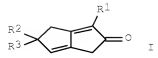


RN 606148-73-6 HCAPLUS
CN Propanedinitrile, 2-(2-phenylethyl)-2-(2-propen-1-yl)- (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 8 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:534178 HCAPLUS Full-text
DOCUMENT NUMBER: 139:350471
TITLE: Palladium-catalyzed [2 + 2 + 1]-intramolecular cycloaddition for the preparation of bicyclo[3.3.0]octa-1.5-dien-3-ones from 1,6-diynes
AUTHOR(S): Grigg, Ronald; Zhang, Lixin; Collard, Simon; Keep, Ann
CORPORATE SOURCE: Molecular Innovation, Diversity and Automated Synthesis (MIDAS) Centre, School of Chemistry, Leeds University, LS2 9JT, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (15), 1902-1903
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:350471
ED Entered STN: 13 Jul 2003
GI



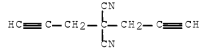
I

AB Palladium-catalyzed [2 + 2 + 1]-cycloaddn. of 1,6-heptadiynes with carbon monoxide furnished bicyclo[3.3.0]octa-1,5-dien-3-ones I (R1 = H; R2 = R3 = H, CO2Me, CO2Et, CN; R1 = Me; R2 = R3 = CO2Me; R1 = H; R2 = CN, R3 = CO2Me) in moderate to good yields.

IT 138024-35-8, Dipropargylmalononitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bicyclooctadienones via palladium-catalyzed intramol. [2 + 2 + 1]-cycloaddn. of alkadiynes)

RN 138024-35-8 HCAPLUS

CN Propanedinitrile, 2,2-di-2-propyn-1-yl- (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 9 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:494750 HCAPLUS Full-text

DOCUMENT NUMBER: 140:16375

TITLE: Regioselective reactions of phenacyl bromide with active methylene compounds

AUTHOR(S): Padmavathi, V.; Balaiah, A.; Reddy, M. Muralidhar; Reddy, D. Bhaskar

CORPORATE SOURCE: Department of Chemistry, Sri Venkateswara University, Tirupati, 517 502, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2003), 42B(6), 1519-1522
CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER: National Institute of Science Communication

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:16375

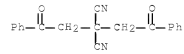
ED Entered STN: 30 Jun 2003

AB The reactivity of phenacyl bromides with active methylene compds. in the presence of alc. KOH, BTEAC (PTC), NaOEt and K2CO3 was studied.

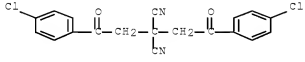
IT 515851-12-4P 629653-22-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective reactions of phenacyl bromides with active methylene compds. for preparation of epoxides and diketones)

RN 515851-12-4 HCAPLUS

CN Propanedinitrile, 2,2-bis(2-oxo-2-phenylethyl)- (CA INDEX NAME)

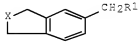


RN 629653-22-1 HCAPLUS
CN Propanedinitrile, 2,2-bis[2-(4-chlorophenyl)-2-oxoethyl]- (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

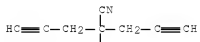
L34 ANSWER 10 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:177679 HCAPLUS Full-text
DOCUMENT NUMBER: 139:149403
TITLE: Highly regio- and chemoselective [2 + 2 + 2] cycloaddition of 1,6-heptadiynes with allenes catalyzed by cobalt complexes
AUTHOR(S): Wu, Ming-Si; Shanmugasundaram, Muthian; Cheng, Chien-Hong
CORPORATE SOURCE: Department of Chemistry, Tsing Hua University, Hsinchu, 300, Taiwan
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (6), 718-719
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:149403
ED Entered STN: 10 Mar 2003
GI



I

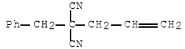
AB The CoI2(PPh3)2/Zn system effectively catalyzes the [2 + 2 + 2] ene-diyne cycloaddn. of 1,6-heptadiynes with allenes in a highly regio- and chemoselective fashion to yield benzene derivs., e.g., I [X = C(COOMe)2, C(CN)2, O, NTs; R1 = alkyl, cycloalkyl], in good to excellent yields.
IT 138024-35-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(indan, isobenzofuran, and indoline derivs. via regio- and chemoselective [2+2+2] cycloaddn. of diynes with allenes catalyzed by cobalt complexes and zinc)
RN 138024-35-8 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propyn-1-yl- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 11 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:158800 HCAPLUS Full-text
DOCUMENT NUMBER: 139:323564
TITLE: Product subclass 1: lead hydrides
AUTHOR(S): Moloney, M. G.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2003), 5, 627-635
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 03 Mar 2003
AB A review on preparation and application of lead hydrides.
IT 6758-00-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and application of lead hydrides)
RN 6758-00-5 HCAPLUS
CN Propanedinitrile, 2-(phenylmethyl)-2-(2-propen-1-yl)- (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

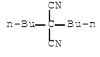
L34 ANSWER 12 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:54465 HCAPLUS Full-text
DOCUMENT NUMBER: 138:401406
TITLE: A facile method for the construction of highly substituted acetonitriles and olefins. Malononitriles as acetonitrile carbanion and alkylidene dianion equivalents
AUTHOR(S): Tsai, Ting-Yueh; Shia, Kak-Shan; Liu, Hsing-Jang
CORPORATE SOURCE: Department of Chemistry, National Tsing Hua

University, Hsinchu, 30013, Taiwan
SOURCE: Synlett (2003), (1), 97-101
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:401406
ED Entered STN: 23 Jan 2003

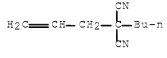
AB The use of malononitrile to facilitate the preparation of highly substituted nitriles, via reductive alkylation/addition, and olefins, via a combination of reductive addition and reductive elimination, is described.

IT 27947-14-4 529508-29-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted nitriles and olefins by using malononitrile and its derivs. as acetonitrile carbanion and alkylidene dianion equivalent through reductive alkylation/addition/elimination reactions)

RN 27947-14-4 HCAPLUS
CN 1,1-Pentanedinitrile, 1-butyl- (CA INDEX NAME)

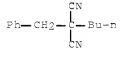


RN 529508-29-0 HCAPLUS
CN Propanedinitrile, 2-butyl-2-(2-propen-1-yl)- (CA INDEX NAME)



IT 529508-27-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted nitriles and olefins by using malononitrile and its derivs. as acetonitrile carbanion and alkylidene dianion equivalent through reductive alkylation/addition/elimination reactions)

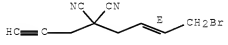
RN 529508-27-8 HCAPLUS
CN Propanedinitrile, 2-butyl-2-(phenylmethyl)- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

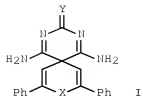
L34 ANSWER 13 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:960934 HCAPLUS Full-text
DOCUMENT NUMBER: 138:337471
TITLE: Novel intramolecular allylindination of terminal alkynes in aqueous media
AUTHOR(S): Salter, Matthew M.; Sardo-Inffiri, Sofia
CORPORATE SOURCE: Department of Chemistry, King's College London, London, WC2R 2LS, UK
SOURCE: Synlett (2002), (12), 2068-2070
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:337471
ED Entered STN: 19 Dec 2002
AB The intramol. cyclization of tethered allyl bromides onto terminal alkynes mediated by metallic indium proceeds smoothly and cleanly in an mixture of THF and water to give unsatd. carbocycles and heterocycles in good yield. The reaction does not proceed efficiently under rigorously anhydrous conditions.
IT 516518-12-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(intramol. cyclization of terminal alkynes in aqueous media using indium catalyst)
RN 516518-12-0 HCAPLUS
CN Propanedinitrile, 2-[(2E)-4-bromo-2-buten-1-yl]-2-(2-propyn-1-yl)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 14 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:885337 HCAPLUS Full-text
DOCUMENT NUMBER: 138:338003
TITLE: 1,5-Diphenyl-3,3-dicyano-1,5-pentanedione: A Synthon for Novel Heterocycles
AUTHOR(S): Padmavathi, V.; Balaiah, A.; Padmaja, A.; Reddy, D. Bhaskar
CORPORATE SOURCE: Sri Venkareswara University, Tirupati, India
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (2002), 177(12), 2791-2798
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:338003
ED Entered STN: 22 Nov 2002
GI



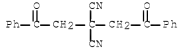
I

AB 1,5-Diphenyl-3,3-dicyano-1,5-pentanedione has been used to incorporate N, O, or S to obtain 1,4-dihydropyridine, 4H-pyran, and 4H-thiopyran derivs., which in turn serve as precursors for novel spiro heterocycles, e.g., I (X = NH, O, S; Y = O, S). All the compds. were characterized by IR and NMR spectral data.

IT 515851-12-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthon for heterocycles)

RN 515851-12-4 HCAPLUS

CN Propanedinitrile, 2,2-bis(2-oxo-2-phenylethyl)- (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 15 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:348362 HCAPLUS Full-text

DOCUMENT NUMBER: 137:63223

TITLE: Catalytic Oxidative Carbonylation of Primary and Secondary Diamines to Cyclic Ureas. Optimization and Substituent Studies

AUTHOR(S): Qian, Fang; McCusker, Jennifer E.; Zhang, Yue; Main, A. Denise; Chlebowski, Mary; Kokka, Michiyo; McElwee-White, Lisa

CORPORATE SOURCE: Department of Chemistry and Center for Catalysis, University of Florida, Gainesville, FL, 32611-7200, USA

SOURCE: Journal of Organic Chemistry (2002), 67(12), 4086-4092
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:63223

ED Entered STN: 10 May 2002

AB W(CO)6-catalyzed oxidative carbonylation of 1,3-propanediamine to the corresponding urea has been examined under a variety of conditions. Following optimization, the Thorpe-Ingold effect on ring closure was studied using 2,2-dialkyl-1,3-propanediamines. For the 2,2-dimethyl- and 2,2-dibutyl-1,3-propanediamines, the yields were increased significantly as compared to that

of the unsubstituted case. The eight-membered cyclic urea 5-butyl-5-ethyl-1,3-diazepan-2-one was formed in 38% yield, while only trace amts. of the cyclic urea were produced from the parent 1,5-pentanediamine. In a study of secondary diamines, yields from the carbonylation of N,N'-dialkyl-2,2-dimethyl-1,3-propanediamines were lower than those obtained from the primary diamines. The main byproducts from secondary diamines were tetrahydropyrimidine derivs., formed by a competitive reaction of the substrate with the oxidant and base.

IT 27947-14-4P, Dibutylmalononitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(catalytic oxidative carbonylation of primary and secondary diamines to cyclic ureas)

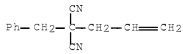
RN 27947-14-4 HCAPLUS

CN 1,1-Pentanedinitrile, 1-butyl- (CA INDEX NAME)

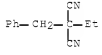
REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 46 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:20668 HCAPLUS Full-text
DOCUMENT NUMBER: 116:20668
ORIGINAL REFERENCE NO.: 116:3639a,3642a
TITLE: Phase transfer catalysis without solvent: selective mono- or dialkylation of malononitrile
AUTHOR(S): Diez-Barra, Enrique; De la Hoz, Antonio; Moreno, Andres; Sanchez-Verdu, Prado
CORPORATE SOURCE: Fac. Quim., Univ. Castilla-La Mancha, Ciudad Real, 13071, Spain
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1991), (10), 2589-92
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:20668
ED Entered STN: 24 Jan 1992
AB Monoalkyl- and sym. or unsym. dialkylmalononitriles have been prepared selectively by phase transfer catalysis in the absence of solvent. Exclusive formation of a particular compound is achieved in all cases except for benzylmalononitrile (79%) and 2-propynylmalononitrile (62%).
IT 6758-08-5P, Allylbenzylmalononitrile 21455-97-0P, Benzylethylmalononitrile 27947-14-4P, Dibutylmalononitrile 28118-33-4P, Diethylmalononitrile 90557-34-9P, Diallylmalononitrile 138024-35-8P, Dipropargylmalononitrile 138024-36-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 6758-00-5 HCAPLUS
CN Propanedinitrile, 2-(phenylmethyl)-2-(2-propen-1-yl)- (CA INDEX NAME)



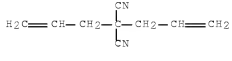
RN 21455-97-0 HCAPLUS
CN 1,1-Propanedinitrile, 1-(phenylmethyl)- (CA INDEX NAME)



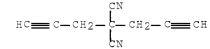
RN 27947-14-4 HCAPLUS
CN 1,1-Pentanedinitrile, 1-butyl- (CA INDEX NAME)

RN 28118-33-4 HCAPLUS
CN Propanedinitrile, 2,2-diethyl- (CA INDEX NAME)

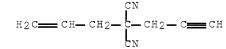
RN 90557-34-9 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propen-1-yl- (CA INDEX NAME)



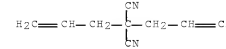
RN 138024-35-8 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propyn-1-yl- (CA INDEX NAME)



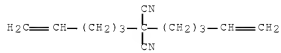
RN 138024-36-9 HCAPLUS
CN Propanedinitrile, 2-(2-propen-1-yl)-2-(2-propyn-1-yl)- (CA INDEX NAME)



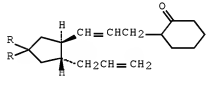
L34 ANSWER 47 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:206611 HCAPLUS Full-text
DOCUMENT NUMBER: 114:206611
ORIGINAL REFERENCE NO.: 114:34831a,34834a
TITLE: The tin hydride reductive decyanation of geminal dinitriles
AUTHOR(S): Curran, Dennis P.; Seong, Churl Min
CORPORATE SOURCE: Dep. Chem., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Synlett (1991), (2), 107-8
CODEN: SYNLES; ISSN: 0936-5214
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:206611
ED Entered STN: 31 May 1991
AB RC(CN)2R1(R = H, alkyl, cycloalkyl; R1 = alkyl, cycloalkyl) are reductively decyanated to the corresponding mononitriles in 75-91% yield on treatment with Bu3SnH and to catalytic amount of 2,2'-azobisisobutyronitrile in refluxing benzene. A mechanism for this reaction is also proposed.
IT 90557-34-9 133682-94-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive decyanation of, with tributyltin hydride)
RN 90557-34-9 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propen-1-yl- (CA INDEX NAME)



RN 133683-94-0 HCAPLUS
CN Propanedinitrile, di-4-pentenyl- (9CI) (CA INDEX NAME)



L34 ANSWER 48 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:477713 HCAPLUS Full-text
DOCUMENT NUMBER: 113:77713
ORIGINAL REFERENCE NO.: 113:13143a,13146a
TITLE: Catalytic palladium-mediated tetraene carbocyclizations: enamine trapping reagents
AUTHOR(S): Takacs, James M.; Zhu, Jingyang
CORPORATE SOURCE: Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588-0304, USA
SOURCE: Tetrahedron Letters (1990), 31(8), 1117-20
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:77713
ED Entered STN: 01 Sep 1990
GI



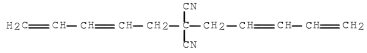
I

AB The Pd-catalyzed carbocyclization of a tetraene substrate in the presence of an enamine effects efficient cyclization of the substrate with concomitant formation of a second carbon-carbon bond via allylation of the enamine. A brief survey of the roles of the reaction medium, ligand, enamine reagent, and to a lesser extent the substrate and palladium catalyst in determining the catalytic efficiency, mode-selectivity, and stereoselectivity of the cyclization is described. For example, reaction of (H2C:CHCH:CHCH2)2CR2 (R = CO2Et, SO2Ph, CN) with 1-pyrrolidino-1-cyclohexene gave cyclopentane derivs. I.

IT 128350-77-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, in the presence of enamine, palladium catalyzed stereoselective intramol.)

RN 128350-77-6 HCAPLUS

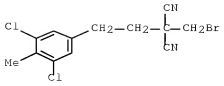
CN Propanedinitrile, di-2,4-pentadienyl- (9CI) (CA INDEX NAME)



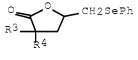
L34 ANSWER 49 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:423695 HCAPLUS Full-text
DOCUMENT NUMBER: 113:23695
ORIGINAL REFERENCE NO.: 113:4107a,4110a
TITLE: Preparation and photochromism of new fulgides and fulgimides with spirocyclic adamantylidene and norbornylidene groups
INVENTOR(S): Tanaka, Takashi; Tanaka, Kenji; Imura, Satoshi; Kida, Yasuji
PATENT ASSIGNEE(S): Tokuyama Soda Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 57 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 351112	A2	19900117	EP 1989-306672	19890630 <--
EP 351112	A3	19910717		
EP 351112	B1	19940928		
R: DE, FR, GB, IT				
US 5130058	A	19920714	US 1989-373100	19890629 <--
JP 02138276	A	19900528	JP 1989-167028	19890630 <--
JP 07042282	B	19950510		

PRIORITY APPLN. INFO.: JP 1988-162663 A 19880701 <--
OTHER SOURCE(S): MARPAT 113:23695
ED Entered STN: 21 Jul 1990
GI For diagram(s), see printed CA Issue.
AB Fifty-nine title compds. I [R1 = (substituted) hydrocarbyl or heterocyclyl; R2 = (substituted) hydrocarbyl; Y = atoms to form (substituted) (hetero)aromatic ring system; Z = atoms to form (substituted) norbornylidene or adamantylidene spiro-system; X = O, NR3; R3 = H, (substituted) hydrocarbyl] were prepared Thus, C-methylation of fulgide II (R2 = H) with K2CO3 and MeI in DMF gave 17% title compound II (R2 = Me); when dispersed in a poly(Me methacrylate) film, its formation-extinction color d. half-life was 3000 cycles, and the thermal half-life at 80° was 1200 h.
IT 127776-10-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of fulgide and fulgimide derivs., in preparation of photochromic substances)
RN 127776-10-7 HCAPLUS
CN Propanedinitrile, 2-(bromomethyl)-2-[2-(3,5-dichloro-4-methylphenyl)ethyl]- (CA INDEX NAME)

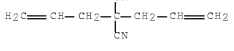


L34 ANSWER 50 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:423555 HCAPLUS Full-text
DOCUMENT NUMBER: 113:23555
ORIGINAL REFERENCE NO.: 113:4079a,4082a
TITLE: Phenylseleno-lactonization of olefinic nitriles promoted by peroxydisulfate ion oxidation of diphenyl diselenide
AUTHOR(S): Tiecco, Marcello; Testaferri, Lorenzo; Tingoli, Marco; Bartoli, Donatella
CORPORATE SOURCE: Fac. Farm., Univ. Perugia, Perugia, 06100, Italy
SOURCE: Tetrahedron (1989), 45(21), 6819-32
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:23555
ED Entered STN: 21 Jul 1990
GI

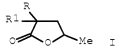


I

AB Oxidation of (PhSe)2 with (NH4)2S2O8 in RCN (R = Me, Et) in the presence of R1CH:CHR2 [R1R2 = (CH2)4; R1 = R2 = Et; R1 = H, R2 = hexyl] gave RCONHCHR1CHR2SePh. A similar reaction using H2C:CHCH2CR3R4CN (R3 = H, Me; R4 = H, Me, Et, Ph, CN) in dioxane gave lactones I in 64-84% yield. The ring closure reaction proceeded through initial formation of hydroxyselenation products.
IT 90557-34-9, 4,4-Dicyano-1,6-heptadiene
RL: RCT (Reactant); RACT (Reactant or reagent)
(selenoetherification of, with di-Ph diselenide)
RN 90557-34-9 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propen-1-yl- (CA INDEX NAME)

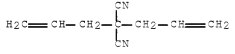


L34 ANSWER 51 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:197997 HCAPLUS Full-text
DOCUMENT NUMBER: 112:197997
ORIGINAL REFERENCE NO.: 112:33465a,33468a
TITLE: Simple synthesis of γ-lactones from olefinic nitriles
AUTHOR(S): Tiecco, Marcello; Tingoli, Marco; Testaferri, Lorenzo; Bartoli, Donatella
CORPORATE SOURCE: Fac. Farm., Univ. Perugia, Perugia, 06100, Italy
SOURCE: Synthetic Communications (1989), 19(16), 2817-24
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:197997
ED Entered STN: 26 May 1990
GI



I

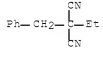
AB Cyclization of pentenonitriles H2C:CHCH2CRR1CN (R = R1 = Me; R = H, R1 = H, Me, Et, Ph) with 50% H2SO4 gave 61-95% δ-lactones I.
IT 90557-34-9, Bis(allyl)malononitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with sulfuric acid, spirolactone from)
RN 90557-34-9 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propen-1-yl- (CA INDEX NAME)



L34 ANSWER 77 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1964:454843 HCAPLUS Full-text
DOCUMENT NUMBER: 61:54843
ORIGINAL REFERENCE NO.: 61:9494c-f
TITLE: Synthetic organic chemistry using liquid ammonia alkali hydroxide. XIX. New barbituric acid synthesis in liquid ammonia-alkali hydroxide. 8. Synthesis of

ethylalkyldiiminobarbituric acid by the condensation of ethylalkylmalononitrile with urea
AUTHOR(S): Shimo, Kotaro; Kawasaki, Toshio
CORPORATE SOURCE: Natl. Defence Acad., Yokosuka, Japan
SOURCE: Kogyo Kagaku Zasshi (1964), 67(4), 574-6
CODEN: KGKZA7; ISSN: 0368-5462
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. CA 58, 9072b. A reaction between 0.05 mole EtHC(CN)2 (I) and 0.055 mole PhCH2Cl in 110 cc. liquid NH3 at room temperature 1.5 hrs. gave 78% EtPhCH2C(CN)2, m. 61-1.5°, after evaporation of NH3, extraction with alc., followed by evaporation of alc. and washing with water. Similarly were prepared following REtC(CN)2 (II) (R, b.p., and % yield given): CH2:CHCH2, 94-5°/21, 68; iso-C5H11, 115-16°/20, 47; Pr, 95-6°/20, 57, from the reactions of I and the corresponding alkyl bromides. A reaction of 0.015 mole II (R = PhCH2) with 0.015 mole urea in the presence of 0.03 mole NaNH2 (or NaOH) in 70 cc. liquid NH3 at room temperature 3 hrs. gave 61% III (R = PhCH2), m. 285-6° (decomposition), after evaporation of NH3, extraction with alc. and subsequent neutralization with AcOH. Also were prepared following III (R, m.p., and % yield given): iso-Am, 268.5-69° (decomposition), 52; CH2:CHCH2, 277.5-78° (decomposition), 57; Pr, 273.5-74° (decomposition), 47, while II (R = H and Ph) did not give the corresponding derivs. III readily gave the corresponding IV when heated with dilute HCl 2 hrs. (R and m.p. given): PhCH2, 206-7.5°; iso-Am, 154.5-55°; allyl, 157-7.5°; and Pr, 146-6.5°.
IT 6731-40-4P, Malononitrile, allylethyl- 21455-97-0P, Malononitrile, benzylethyl- 90196-82-0P, Malononitrile, ethylpropyl- 91010-29-6P, Malononitrile, ethylisopentyl-
RL: PREP (Preparation)
(preparation of)
RN 6731-40-4 HCAPLUS
CN Malononitrile, allylethyl- (7CI, 8CI) (CA INDEX NAME)

RN 21455-97-0 HCAPLUS
CN 1,1-Propanedinitrile, 1-(phenylmethyl)- (CA INDEX NAME)



RN 90196-82-0 HCAPLUS
CN 1,1-Butanedinitrile, 1-ethyl- (CA INDEX NAME)

RN 91010-29-6 HCAPLUS
CN 1,1-Pentanedinitrile, 1-ethyl-4-methyl- (CA INDEX NAME)

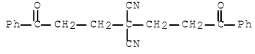
L34 ANSWER 78 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1964:93628 HCAPLUS Full-text
DOCUMENT NUMBER: 60:93628
ORIGINAL REFERENCE NO.: 60:16389e-f
TITLE: Influence on neurotropic virus infections of the mouse by dinitrile compounds
AUTHOR(S): Bock, M.; Distelmaier, A.
SOURCE: Med. Chemie, Abhandl. Med. Chem. Forschungsstaetten Farbenfabriken Bayer (1963), 7, 609-28
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB In chemotherapeutic tests on the encephalomyelitis-, poliomyelitis (type II), and encephalomyocarditisvirus infections of mouse the effect of malonitrile, described by Szanto and Felsenfeld (CA 44, 1198e) for the Lansing virus, could not be proved. The influence on the progress of the malady with other less toxic dinitrile compds. could likewise not be found. They are also inactive on exptl. brain infections with neurotropic virus (choriomeningitis, rabies, and west-Nile virus).
IT 28118-33-4, Malononitrile, diethyl-
(virus infection and)
RN 28118-33-4 HCAPLUS
CN Propanedinitrile, 2,2-diethyl- (CA INDEX NAME)

L34 ANSWER 79 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1964:52504 HCAPLUS Full-text
DOCUMENT NUMBER: 60:52504
ORIGINAL REFERENCE NO.: 60:9194c-e

TITLE: The thermal reversibility of the Michael reaction. I. Nitriles
AUTHOR(S): Allen, C. F. H.; Happ, G. P.
CORPORATE SOURCE: Rochester Inst. of Technol., Rochester, NY
SOURCE: Canadian Journal of Chemistry (1964), 42(3), 641-9
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001

AB Michael adducts of nitriles and α,β-unsatd. ketones have been found generally to undergo 2 or more kinds of thermal reversibility upon being heated to moderate temps. When the products are those from which the adduct was prepared, the dissociation is termed "normal," whereas the "abnormal" route gives an α,β-unsatd. nitrile and a Me ketone. The scope and generality of the reversibility are described in 3 papers. The 1st deals with 31 ketonic nitriles, the 2nd with nitroketones, and the last with diketones and acidic derivs. Allowing the materials to decompose thermally in the heated inlet of a mass spectrometer permits a direct study of thermal reaction mixts. and it affords data the interpretation of which gives an indication of the products present, many of which may not have been previously expected. Identification of products is confirmed by comparison of the mass spectra with those of reference compds. Under favorable conditions, such products can be isolated from independent decomposition reactions and their identities further confirmed by classical chemical methods. Both operations have been done often enough to show the general application of the mass spectrometer for this purpose. Thus laborious laboratory sepns. may be avoided. In 2 instances the 4 major products from both paths were isolated, identified, and quant. determined

IT 13993-28-7, Malononitrile, bis(2-benzoylethyl)-
(thermal decomposition of)
RN 13993-28-7 HCAPLUS
CN 1,1-Butanedinitrile, 4-oxo-1-(3-oxo-3-phenylpropyl)-4-phenyl- (CA INDEX NAME)



L34 ANSWER 80 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:474844 HCAPLUS Full-text
DOCUMENT NUMBER: 59:74844
ORIGINAL REFERENCE NO.: 59:13819h,13820a-c
TITLE: Bis(2-bromoalkyl)malononitriles by addition of dibromomalononitrile to alkenes
AUTHOR(S): Roland, J. R.; Little, E. L., Jr.; Winberg, H. E.
CORPORATE SOURCE: E. I. du Pont de Nemours & Co., Wilmington, DE
SOURCE: Journal of Organic Chemistry (1963), 28(10), 2809-11
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001

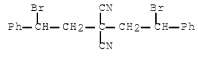
GI For diagram(s), see printed CA Issue.

AB cf. CA 52, 18429a; Torssell and Dahlqvist, CA 57, 5842c. Br2C(CN)2 (I) (22.4 g.) heated 16 hrs. at 150° and 1000 atmospheric with C2H4 and 150 ml. C6H6 in a stainless steel pressure vessel gave 20 g. (BrCH2CH2)2C(CN)2 (II), m. 59-60° (C6H6). In the presence of 0.5 g. Cu, only 4.0 g. II was obtained. I (22.4 g.) heated 3 hrs. at 80° with 50 ml. 1-hexene and 0.5 g. Cu gave 39 g. of a mixture of meso and racemic isomers of (Bu CH BrCH2)2C(CN)2, from which were separated 14.9 g. higher-melting isomer (III), m. 124-5°(alc. or hexane), and 20.8 g. lower-melting isomer (IV), m. 76-7° (hexane or alc.). The reaction with 1-hexene did not proceed without an initiator, but Bz2O2, azobis (α,γ-dimethylvaleronitrile), FeCl3, SnCl4, and AlCl3 also catalyzed it. A free radical mechanism was proposed for initiation by all but SnCl4 and AlCl3, for which an ionic mechanism was suggested. I heated with styrene and Cu gave a mixture (V), m. 134-40° (alc.), of stereoisomers of (PhCHBrCH2)2C-(CN)2. I treated at about 0° with 3-methylenecyclobutanecarbonitrile and Cu gave 56% 1,3-bis(1-bromo-3-cyanobutyl)-2,2dicyanopropane, m. 192-4° (aqueous Me2CO). II (1.0 g.) heated with 3 ml. concentrated H2SO4 and 2.3 ml. H2O gave 0.33 g. VI (R : H) (VII), m. 108.5-8.8°. Similarly, IV gave 52% VI (R : Bu) (VIII), m. 102.5-3° (hexane), and III gave another stereoisomer, m. 117-18° (EtOH) of VIII. Neither II nor IV reacted with AgNO3. IV did not react with NaI in Me2CO. Nuclear magnetic resonance peaks were given for II-V and VII.

IT 72228-00-3P, Malononitrile, bis(β-bromophenethyl)-
89694-74-6P, Malononitrile, bis(2-bromoethyl)-
RL: PREP (Preparation)
(preparation of)

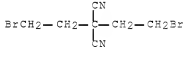
RN 72228-00-3 HCAPLUS

CN 1,1-Propanedinitrile, 3-bromo-1-(2-bromo-2-phenylethyl)-3-phenyl- (CA INDEX NAME)



RN 89694-74-6 HCAPLUS

CN 1,1-Propanedinitrile, 3-bromo-1-(2-bromoethyl)- (CA INDEX NAME)



L34 ANSWER 81 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1962:73004 HCAPLUS Full-text

DOCUMENT NUMBER: 56:73004

ORIGINAL REFERENCE NO.: 56:14026c-i

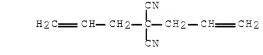
TITLE: Solvent catalyzed alkylations of active methylene groups in liquid ammonia

AUTHOR(S): Shimo, Kotaro; Wakamatsu, Shigeru; Inoue, Tadao

CORPORATE SOURCE: Defence Acad., Yokosuka, Japan

SOURCE: Journal of Organic Chemistry (1961), 26, 4868-71
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 56:73004
ED Entered STN: 22 Apr 2001
AB A new modification of the alkylation reaction was investigated. It was found that some active methylene compds., such as $CH_2(CN)_2$ (I), cyanoacetamide (II), and substituted cyanoacetamide, could be successfully alkylated with alkyl halide to form the corresponding C-alkylation products without the condensing agent in liquid NH_3. The high yields were generally obtained with very reactive benzyl and allyl halides. Six new compds. were prepared in this investigation. The reactions were carried out by 2 general methods: (A) the use of a pressure vessel at room temperature, and (B) the reaction at atmospheric pressure below the b.p. of liquid NH_3. Method A. I (3.3 g.) and 12.7 g. $PhCH_2Cl$ (IIa) in a glass pressure vessel treated with 50 cc. liquid NH_3, the mixture left 24 hrs. at room temperature, the NH_3 evaporated, the remaining solids washed and recrystd. gave 9.1 g. dibenzylmalononitrile (IIb). Method B. Allyl bromide (III) (36.3 g.) added dropwise to 12.6 g. II in 150 cc. liquid NH_3 in 1 hr. at -50°, the mixture stirred 3 hrs., evaporated, the residue washed with H_2O, the solids dissolved in hot H_2O, left and at room temperature precipitated 10.5 g. 2,2-diallylcyanoacetamide (IV). 2-Allylcyanoacetamide (IVa) was isolated from the filtrate. Method B. 2-Acetamidocyanoacetamide (IVb) (7.1 g.) and 150 cc. liquid NH_3treated at -50° with 7.8 g. EtI, evaporated, and the product crystallized gave 6 g. 2-acetamido-2-ethylcyanoacetamide (V). The following alkylation of malononitriles and cyanoacetamides with alkyl halides was thus accomplished (compound alkylated, alkyl halide, method, product, and % yield given): I, III, B, $(CH_2{:}CHCH_2)_2C(CN)_2$ (VI), 91; I, IIa, A, IIb, 74; I, IIa, B, IIb, 75; I, EtI, A, $Et_2C(CN)_2$ (VII), 44; I, EtI, B, VII, 72; II, III, B, IVa, 43 (IV, 21); II, EtI, B, EtCH(CN)CONH2 (VIII), 24. The alkylation of phenyl- and acetamidocyanoacetamides with alkyl halides in liquid ammonia gave the following results [PhCH(CN)-CONH2 (VIIIa) or IVb, alkyl halide, method, R and R1 of RR1C(CN)CONH2, compound number, and % yield given]: VIIIa, III, B, $CH_2{:}CHCH_2$, Ph, IX, 91; VIIIa, IIa, B, $PhCH_2$, Ph, X, 74; VIIIa, EtI, B, Et, Ph, XI, 69; VIIIa, EtI, A, Et, Ph, XI, 45; VIIIa, EtBr, A, Et, Ph, XI, 43; VIIIa, EtBr, B, H, Ph, VIIIa, 79; VIIIa, PrBr, A, Pr, Ph, XII, 42; VIIIa, PrBr, B, H, Ph, VIIIa, 86; VIIIa, iso-PrBr, A, iso-Pr, Ph, XIII, 40; VIIIa, iso-PrBr, B, H, Ph, VIIIa, 94; VIIIa, BuBr, A, Bu, Ph, XIV, 33; VIIIa, BuBr, B, H, Ph, VIIIa, 91; VIIIa, iso-BuBr, A, iso-Bu, Ph, XV, 30; IVb, III, B, $CH_2{:}CHCH_2$, AcNH, XVI, 91; IVb, IIa, B, $PhCH_2$, AcNH, XVII, 71; IVb, IIa, A, $PhCH_2$, AcNH, XVII, 65; IVb, EtI, B, Et, AcNH, V, 71; IVb, EtI, A, Et, AcNH, V, 41; IVb, EtBr, B, Et, AcNH, V, 21; IVb, PrBr, A, Pr, AcNH, XVIII, 21. The following m.ps. were obtained (compound number and m.p. given): VI, 36°; IIb, 130-1°; VII, 46-7°; IVa, 101-4°; IV, 128-9°; VIII, 112.5-13.5°; IX, 115-16°; X, 135.5-6.0°; XI, 117-17.5°; XII, 115-16°; XIII, 125.5-6.5°; XIV, 127.5°; XV, 97.5-100°; XVI, 194-8°; XVII, 205-6°; V, 205°; XVIII, 210-11°.
IT 28118-33-4P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Solvent catalyzed alkylations of active methylene groups in liquid ammonia)
RN 28118-33-4 HCAPLUS
CN Propanedinitrile, 2,2-diethyl- (CA INDEX NAME)

IT 90557-34-9P, Malononitrile, diallyl-
RL: PREP (Preparation)
(preparation of)
RN 90557-34-9 HCAPLUS
CN Propanedinitrile, 2,2-di-2-propen-1-yl- (CA INDEX NAME)



L34 ANSWER 82 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:45525 HCAPLUS Full-text
DOCUMENT NUMBER: 56:45525
ORIGINAL REFERENCE NO.: 56:8548c-i,8549a
TITLE: Alkylation reactions in dimethyl sulfoxide
AUTHOR(S): Bloomfield, Jordan J.
CORPORATE SOURCE: Univ. of Illinois, Urbana
SOURCE: Journal of Organic Chemistry (1961), 26, 4112-15
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB Malononitrile (I) (16.5 g.) in 45 ml. di, methyl sulfoxide (II) added in 15 min. to a slurry of 12 g-NaH in 75 ml. II, the mixture stirred a further 15 min., 63.2 g. PhCH2Cl added in 20 min., the mixture stirred 8.5 hrs. at room temperature, poured into H2O, and the product crystallized gave 39 g. dibenzylmalononitrile, m. 131.8-2.5° (alc.). Similarly 68.5 g. BuBr and I in II stirred a total of 2.5 hrs. gave 2 fractions: (1) 5.8 g., b18 118-31° n25D 1.4291, which vapor phase chromatography showed to contain 11:12 ratio of 2 components, and (2) 30.8 g., b18 131-41°, n24D 1.4310, consisting of dibutylmalononitrile, n24D 1.4313, when purified. Reaction of 14 g. I with excess MeI under the same conditions gave 12 g. dimethylmalononitrile, b5 52°, n25D 1.398, m. 33.7-4.4°. Under the conditions previously described the reaction mixture containing diisopropylmalononitrile (III) turned brown when the halide was added. When 0.75 mole NaH and 0.75 mole iso-PrBr were used with 0.5 mole I, the contents set to a paste when one-third of the mixture had been added; the remaining halide and an addnl. 50 ml. II added, the mixture heated 2 hrs., 20 ml. AcOH added in 100 ml. ligroine, cooled, poured into 100 ml. H2O, extracted with Et2O, washed, the solvent evaporated, and the product distilled gave 2 fractions: (1) 1.8 g., b18-20 88-95°, 2 components in the ratio 5:7 by vapor phase chromatography, (2) 24 g., b18-20 95-102°, with 2 components 1:8. Redistn. at atmospheric pressure gave 6 fractions. The first 2 fractions contained as many as 5 components. The last fraction was III, b. 211-13° n24D 1.4287. To a slurry of 6 g. NaH in 150 ml. II was added 25 g.

2,4-pentanedione (IV), after 30 min. 40 g. MeI added in 20 min., after stirring 0.5 hr. 6 g. Nail added, and after 15 min. 40 g. more MeI. This process was repeated, the solution stirred an addnl. 9 hrs., 150 ml. Et2O added, and the product distilled to give 20.3 g. 3,3-dimethyl-2,4-pentanedione (V), b. 168-72°, n23D 1.4289. BuBr (83.5 g.) added in 20 min. to 25 g. IV, 12 g. NaH, and 100 ml. II, 100 ml. C6H6 added, the solution refluxed 0.5 hr., treated with H2O, extracted with Et2O, and the product distilled gave 4 fractions. Fraction 4 in pentane cooled to -80° gave a product, m. 11-12° which distilled at 20 mm. gave 9.3 g. 3,3-dibutyl-2,4-pentanedione (VI), b. 136-42°, n24D 1.4468. Anal. pure VI was prepared by treatment with a saturated solution of Cu(II) acetate, and the organic residue distilled at 120° n30D 1.4440; 2,4-dinitrophenylhydrazone m. 244.3-5.0° (decomposition). Vapor phase chromatography of the residues indicated the presence of 5 components. The major component was 3-butyl-2,4-pentanedione, b. 100°, n30D 1.4338; Cu chelate m. 183-5°; 2,4-dinitrophenylhydrazone m. 195.4-6.6° (EtOAc-alc.). PhCH2Cl (63.2 g.) added in 20 ml. to 12 g. NaH and 26 g. IV in 100 ml. II, left 2.5 hrs. at room temperature, warmed 1 hr. on a steam bath, poured into H2O, extracted with Et2O, evaporated, and the product collected gave product, C19H20O2, m. 113.2-13.4° (C6H6ligroine); 2,4-dinitrophenylhydrazone m. 252-3.5° (decomposition) EtOAc). Cooling of the mother liquors gave another 2.5% product; the solvent evaporated and the residue fractionated at 0.1 mm. gave 6 fractions. After distillation at atmospheric pressure, infrared spectra and vapor phase chromatography showed the 1st fraction contained a mixture of PhCH2OH and PhCH2OAc. Fractions 3 and 4 treated with saturated Cu(OAc)2 gave a Cu chelate of 3-benzyl-2,4-pentanedione, m. 203-5°. A portion of the original fraction 3 gave the 2,4-dinitrophenylhydrazone, m. 200.3-2.0° (EtOAc-alc.). The 5th fraction gave 1,1-dibenzylacetone; 2,4-dinitrophenylhydrazone, orange needles, m. 124.6-5.8°. The other components of the reaction were not identified.

IT 27947-14-4P, Malononitrile, dibutyl-
RL: PREP (Preparation)
(preparation of)

RN 27947-14-4 HCAPLUS

CN 1,1-Pentanedinitrile, 1-butyl- (CA INDEX NAME)

L34 ANSWER 83 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:	1961:48311 HCAPLUS Full-text
DOCUMENT NUMBER:	55:48311
ORIGINAL REFERENCE NO.:	55:9270e-i
TITLE:	Synthesis of aliphatic thiocarbonic acid amides (between 4 and 10 carbons)
AUTHOR(S):	Schultz, Otto E.; Ranke, Ursula
CORPORATE SOURCE:	Univ. Kiel, Germany
SOURCE:	Archiv der Pharmazie und Berichte der Deutschen Pharmazeutischen Gesellschaft (1961), 294, 82-9 CODEN: APBDAJ; ISSN: 0376-0367
DOCUMENT TYPE:	Journal
LANGUAGE:	Unavailable
OTHER SOURCE(S):	CASREACT 55:48311

ED Entered STN: 22 Apr 2001

AB Refluxing 2.35 g. AcNH2 in 40 g. xylene with 2.76 g. K3PS4 1 hr., extracting the mixture with xylene, and crystallizing the xylene residue from Et2O gave 80% MeCSNH2. To 10 g. Me2CHCH2CN in a bomb tube at -80° was added 10 ml. liquid H2S and 10 ml. HBr, the mixture kept 6 days at 32°, the residue alkalized with 10% NH3, extracted with Et2O, and the residue of the extract crystallized to give 56% Me2CHCH2CSNH2, m. 60-1° (Et2O-pentane). When the reaction was performed with 10 ml. HI 5 days at 50°, the yield was 71%. Similarly, Me2CHCN with HBr gave 77% and with HI 80% Me2CHCSNH2, m. 75°. CH2(CN)2 (I) (5 g.) in 50 ml. alc. was treated with 10 ml. NH3-saturated alc. at -10° then with H2S 3-4 hrs. at -10°, the mixture allowed to stand under H2S 1 day at room temperature, warmed 4-5 hrs. at 50°, cooled, and filtered to give 36% CH2(CSNH2)2, m. 215° (H2O). When the reaction was performed in 200 ml. alc. the yield was 80% and in 80 ml. alc. with 10 drops Et3N 70%. I (13.2 g.) in 40 g. absolute Et2O treated with 8.5 g. Na in 375 ml. alc. then with 43.6 g. EtBr, the mixture refluxed 5 hrs., cooled, filtered, and the residue distilled gave 68% Et2C(CN)C(OEt):NH (II), b17 92°. Et2C(CONH2)2 (8 g.) was mixed with 16 g. P2O5, heated to 210°, and the liquid distilled in vacuo to give 67% Et2C(CN)2 (III). III (3 g.) in 120 ml. alc. treated with NH3 and H2S as above or 1 g. in 40 ml. C6H6 with 10 drops Et3N gave 100% Et2C(CN)CSNH2 (IV), m. 133° (ligroine), also obtained in 91% yield from 10 g. II in 30 g. alc. with NH3 and H2S as above or in 48% yield by treating 4 g. III in 160 ml. alc. containing 0.2 g. K at -10° with H2S 3-4 hrs. and then as above after removing 25% Et2C(CN)CSOEt (V), b14 97-100°, by distillation V was hydrolyzed with alc. NH3 to IV. Treating III with HBr and H2S as above gave 93% Et2C(CSNH2)2, m. 195° (xylene), also prepared from II in 51% and from IV in 77% yield.

IT 28118-33-4P, Malononitrile, diethyl-
RL: PREP (Preparation)
(preparation of)

RN 28118-33-4 HCAPLUS

CN Propanedinitrile, 2,2-diethyl- (CA INDEX NAME)

L34 ANSWER 84 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1960:103193 HCAPLUS Full-text

DOCUMENT NUMBER: 54:103193

ORIGINAL REFERENCE NO.: 54:19579d-f

TITLE: α-Phenyllevulinic acid and derivatives. II

AUTHOR(S): Eskola, Salli; Hakkinen, Hertta Maija; Niemi, Eeva Liisa

CORPORATE SOURCE: Univ. Helsinki

SOURCE: Suomen Kemistilehti B (1959), 32B, 105-8
CODEN: SUKBAJ; ISSN: 0371-4101

DOCUMENT TYPE: Journal

LANGUAGE: German

ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

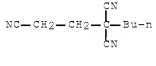
AB cf. CA 51, 288b. α-Phenyllevulinic acid (I) (m. 127°) (100 g.) and 100 ml. AcCl was heated to distil excess AcCl until the flask contents reached 120°

and the residue washed with H2O to yield 90.0 g. crude α-phenyl-Δα,β-angelicalactone (II), m. 52-2.5° (75% EtOH). Alternatively, 11 g. I and 0.5 g. 89% H3PO4 was distilled in vacuo to give 7.9 g. crude II, m. 52-2.5° (75% EtOH). H evidently resulted from the spontaneous rearrangement of MeC:CH.CHPh.CO.O. II was reduced by the Clemmensen method (10 g. II, 3 g. HgCl2 in 120 ml. H2O, 60 g. Zn, 180 ml. concentrated HCl, 1.5 hrs., 25 ml. concentrated HCl, 10 hrs., 25 ml. HCl, 20 hrs.) to 6.9 g. α-phenyl-γ-valerolactone, b3.5 170-1°, and 1.4 g. α-phenylvaleric acid, m. 45-7° (ligroine).

IT 99168-06-6P, 1,3,3-Heptanetricarbonitrile
RL: PREP (Preparation)
(preparation of)

RN 99168-06-6 HCAPLUS

CN 1,1,3-Propanetricarbonitrile, 1-butyl- (CA INDEX NAME)



L34 ANSWER 85 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1960:103192 HCAPLUS Full-text

DOCUMENT NUMBER: 54:103192

ORIGINAL REFERENCE NO.: 54:19578h-i,19579a-d

TITLE: Comparative kinetic investigations on the activation of the methylene group by oxygen- and sulfur-containing groups. The kinetics of the Michael addition

AUTHOR(S): Schmidt, Ulrich; Kubitzek, Harry

CORPORATE SOURCE: Univ. Freiburg, Freiburg, Germany

SOURCE: Chemische Berichte (1960), 93, 866-72
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

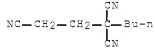
AB The Michael addition of BuCH(CN)2 (I), BuCH(CO2Et)2 (II), BuCH(CN)CO2Et (III), BuCH(CO2Et)COSEt (IV), AcBuCHCO2Et (V), and BuCH(COSEt)2 (VI) to CH2: CHCN (VII) in nonaq. media in the presence of catalytic amts. of strong bases proceeded as a pseudomonomol. reaction. The same activation energy of 10 ± 0.7 kcal./mole was found for the addition reactions of compds. I-VI to VII. To 50 cc. 0.3M appropriate methylene derivative in 1:10 dioxane-Me3COH was added 50 cc. Me3COK in Me3COH, the mixture adjusted to the desired temperature, treated with stirring with 50 cc. 0.3M VII in dioxane-Me3COH, aliquots were withdrawn at certain time intervals and added to a measured volume of 0.15M alc. PhCH2SH (about 25% excess), the mixture was treated with a few drops 0.5N NaOEt-EtOH, acidified after 2 min. with 2 cc. AcOH, diluted with 50 cc. EtOH, and back-titrated with 0.05N iodine-KI to give the rate data for the reaction. The temperature dependence of the rate of the addition reaction was determined in this manner (reactant, M catalyst concentration, and kl min.-1 at 15, 20, 25, and 30° given): I, 0.0003, 0.135, 0.180, 0.237, -; II, 0.0003, 0.089, 0.120, 0.160, -; III, 0.0003, -, 0.0125, 0.0169, 0.0223; IV, 0.002, 0.031, 0.0414, 0.0556, -; V, 0.0158, 0.075, 0.099, 0.135, -; VI, 0.02, 0.00564, 0.00805, 0.0096, 0.0136. BuCH(CN)CONH2 (48 g.) and 29 g. PCl5 heated slowly in vacuo to 180°, the crude distillate, b35-40 135-40°,

dissolved in Et2O, and the solution washed with aqueous NaHCO3 and H2O and worked up in the usual manner gave 29 g. I, b0.01 46-8°, n20D 1.4292. BuCH(CO2H)CO2Et (194 g.) treated with PCl5 in Et2O, and the crude product treated with EtSH and C5H5N in CHCl3 at 0° gave 194 g. IV, b0.8 90-1°, n22D 1.4608. BuCH(COCl)2 with EtSH and C5H5N in CHCl3 gave 38% VI, b0.05 97-8°, n21D 1.5010. The appropriate methylene derivative (II-VI) (0.1 mole) in 50 cc. Me3COK in dioxane-Me3COH treated with stirring slowly with 0.11 mole VII, the mixture treated after 2-3 hrs. with a small amount dry HCl and evaporated, and the residue dissolved in Et2O, washed, and worked up gave the corresponding addition product (b.p./mm., nD/temperature, and % yield given): Bu(NCCH2CH2)C(CN)CO2Et, 115-16°/0.02, 1.4488/22°, 70; Bu(NCCH2CH2)CAcCO2Et, 138-40°/0.2, 1.4530/20°, 62; Bu(NCCH2CH2)C(CO2Et)COSEt, 125-8°/0.02, 1.4760/23°, 84; Bu(NCCH2CH2)C(COSEt)2, 166-8°/0.1, 1.5159/17.5°, 60; Bu(NCCH2CH2)C(CN)2, - (m. 55.5°), -, 65.

IT 99168-06-6P, 1,3,3-Heptanetricarbonitrile
RL: PREP (Preparation)
(preparation of)

RN 99168-06-6 HCAPLUS

CN 1,1,3-Propanetricarbonitrile, 1-butyl- (CA INDEX NAME)



L34 ANSWER 86 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1959:105201 HCAPLUS Full-text

DOCUMENT NUMBER: 53:105201

ORIGINAL REFERENCE NO.: 53:18859f-h

TITLE: Some dialkyl substituted malonothioamides

AUTHOR(S): Vega, Carlos M.

CORPORATE SOURCE: Univ. Buenos Aires

SOURCE: Revista de la Asociacion Bioquimica Argentina (1958), 23, 212-22
CODEN: RABAAO; ISSN: 0004-4768

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

AB Et2C(CN)2 (I), b3 47-50°, m. 42-3°, was prepared in 76% yield by dehydration of NCCEt2CONH2 with P2O5. Iso-PrEtC(CN)CONH2 with P2O5 gave 60% iso-PrEtC(CN)2 (II), b2 45° (2 mm. Hg). I in absolute EtOH with K at -10°, then H2S, followed by stirring and warming to below 50°, gave 25% Et2C(CN)CSNH2, m. 121-3°. The dithioamide could not be prepared by this method. Prolonged heating of a II-alc.-K metal-H2S mixture yielded crystals m. 135-7°, believed to be a mixture of the mono- and dithioamides.

IT 28118-33-4P, Malononitrile, diethyl-
RL: PREP (Preparation)
(preparation of)

RN 28118-33-4 HCAPLUS

CN Propanedinitrile, 2,2-diethyl- (CA INDEX NAME)

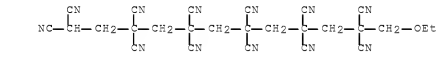
L34 ANSWER 87 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:61030 HCAPLUS Full-text
DOCUMENT NUMBER: 52:61030
ORIGINAL REFERENCE NO.: 52:10953h-i,10954a-g
TITLE: Vinylidene cyanide. IX. Reaction of polyvinylidene cyanide with compounds containing a single active hydrogen atom
AUTHOR(S): Westfahl, J. C.
CORPORATE SOURCE: B. F. Goodrich Research Center, Brecksville, O.
SOURCE: Journal of the American Chemical Society (1958), 80, 871-4
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:61030
ED Entered STN: 22 Apr 2001
AB cf. C.A. 51, 1116f. The base-catalyzed reaction of low mol. weight poly(vinylidene cyanide) with active H compds. containing a single H atom was studied. EtOH (50 cc.) added during 7 min. with stirring to 143 cc. solution containing approx. 39 g. CH2: C(CN)2 (I), AcOH, and PhCl [obtained by flash distillation of the pyrolysis product of di(acetyl cyanide) (cf. U.S. 2,663,726, C.A. 49, 4711a)] below 30°, the mixture stirred 35 min., diluted with 200 cc. hexane, stirred 10 min., and filtered with suction, and the residue washed with hexane and dried at 60°/0.01 yielded 37.6 g. EtO[CH2C(CN)2]nH (n = average 6) (II). Cl(CH2)2OH (15 cc.) added with stirring to 10 cc. 91.35% I in 20 cc. C6H6, stirred 1.5 hrs. without cooling, kept at room temperature overnight, diluted with 50 cc. hexane, stirred, and filtered gave 10.16 g. Cl(CH2)2O[CH2C(CN)2]nH (n = average 7). EtOH (10 cc.) in 10 cc. C6H6 added during 8 min. with stirring to 8.8 cc. 90% I and 40 cc. C6H6, stirred 0.5 hr., and evaporated in vacuo, the residual II stirred with 40.0 g. Me2CHNO2, b. 118-18.5°, n25D 1.3925, d25 0.991, treated at 23° with stirring during 30 sec. with 10.0 cc. piperidine, stirred 15 min., cooled, diluted with 100 cc. cold H2O, 8 cc. concentrated HCl, and 100 cc. Et2O, and filtered, the aqueous layer extracted with Et2O, and the combined Et2O solns. dried and evaporated in vacuo yielded 13.03 g. Me2C(NO2)CH2CH(CN)2, pale yellow, m. 82-3° (EtOH). EtCH(CO2Et)2 (III) (56.46 g.) added to 2.30 g. Na in 35 cc. EtOH, the EtOH removed in vacuo, the residue stirred with 7.81 g. II, heated 25 min. at 50-60°, cooled, treated with 100 cc. H2O, 10 cc. concentrated HCl, and 50 cc. Et2O, and filtered with Filter-aid, the aqueous layer of the filtrate extracted with Et2O, the combined Et2O solns. evaporated, and the residue distilled gave 35.44 g. unchanged III and left 21.97 g. (crude) (EtO2C)2CEtCH2CH(CN)2 (IV), m. 55.4-6.5° (EtOH). IV (5.0 g.) and 5.00 g. NaOH in 50 cc. H2O refluxed 17 hrs., concentrated to approx. 25 cc., cooled, adjusted to pH 6 with HCl, filtered, treated with 25 cc. concentrated HCl, refluxed 4 hrs., and evaporated, the residue extracted with boiling Et2O, and the extract dried and evaporated yielded 2.55 g. HO2CCHEt(CH2)2CO2H which refluxed with AcCl and then treated with p-MeC6H4NH2 gave 38.7% mixed isomeric N-(p-tolyl)-α-ethylglutaramic acid (V), m. 148-8.5°. V refluxed gently at atmospheric pressure gave N-(p-tolyl)-α-ethyl-glutarimide, m. 96-7°. CH2(CO2Et)2 (160 g.) containing 0.1 equivalent II

treated with 8.1 cc. pyridine, stirred 10 min., heated 2 hrs. at 50-60°, kept at room temperature overnight, diluted with 100 cc. H2O and 10 cc. concentrated HCl, and processed in the usual manner gave 144.7 g. unchanged CH2(CO2Et)2 and 15.1 g. partly crystalline material which recrystd. from EtOH gave 5.75 g. bis compound, C15H16N4O4, m. 143.5-4.5°; the mother liquor evaporated, and the residue distilled gave 3.31 g. (EtO2C)2CHCH2CH(CN)2 (VI), b0.02 115-27°, and 4.79 g. residue. VI (3.31 g.), 4.0 g. NaOH, and 30 cc. H2O refluxed 23 hrs., cooled, acidified, filtered, and extracted with Et2O, and the extract worked up gave 0.87 g. [(HO2C)2CH]2CH2, m. 173° (with gas evolution), which heated at 180-5° gave CH2(CH2CO2H)2, m. 94-7° (C6H6). Pyridine (4.1 cc.) added with stirring to 4.40 g. II, 10.12 g. C12H25SH, and 40 cc. C6H6, heated 0.5 hr. at 50-60°, cooled, treated with 50 cc. H2O and 5 cc. concentrated HCl, and filtered, and the C6H6 layer worked up gave 13.90 g. (crude) C12H25SCH2CH(CN)2 (VII), m. 40.5-1.5° (hexane). VII (2.00 g.), 15 cc. concentrated HCl, and 10 cc. glacial AcOH refluxed 16 hrs., cooled, and diluted with H2O gave 1.47 g. (crude) C12H25S(CH2)2CO2H (VIII), m. 59-61.5° (hexane). Na salt of VIII in H2O oxidized with KMnO4 gave C12H25SO2(CH2)2CO2H, m. 135-7°. II (3.90 g.), 6.21 g. PhCH2SH, and 3.96 g. pyridine in 40 cc. C6H6 gave in the usual manner 5.14 g. PhCH2SCH2CH(CN)2 (IX), m. 47.5-8.5° (C6H6-hexane). IX (1.00 g.) refluxed 16.5 hrs. with 15 cc. concentrated HCl and 5 cc. H2O gave 0.67 g. PhCH2S(CH2)2CO2H, m. 81.2-82° (hexane), which oxidized as the Na salt in H2O with KMnO4 gave 57.4% PhCH2SO2(CH2)2CO2H, m. 177-8°.

IT 114598-88-8P, 1,1,3,3,5,5,7,7,9,9,11,11-Dodecanedodecacarbonitrile, 12-ethoxy- 119925-88-1P, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecane-tetradecacarbonitrile, 14-(2-chloroethoxy)-
RL: PREP (Preparation)
(preparation of)

RN 114598-88-8 HCAPLUS

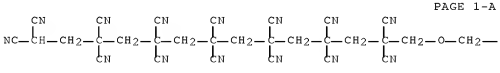
CN 1,1,3,3,5,5,7,7,9,9,11,11-Undecanedodecacarbonitrile, 1-(ethoxymethyl)- (CA INDEX NAME)



RN 119925-88-1 HCAPLUS

CN 1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tridecanetetradecacarbonitrile, 1-[(2-chloroethoxy)methyl]- (CA INDEX NAME)

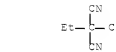
PAGE 1-A



—CH_2Cl

L34 ANSWER 88 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1952:23336 HCAPLUS Full-text
DOCUMENT NUMBER: 46:23336
ORIGINAL REFERENCE NO.: 46:3944f-i,3945a
TITLE: Some applications of deuterium in the study of decomposition mechanisms of organic compounds
AUTHOR(S): Wall, Leo A.; Moore, Walter J.
CORPORATE SOURCE: Natl. Bur. Standards, Washington, DC
SOURCE: Journal of Physical and Colloid Chemistry (1951), 55, 965-74
CODEN: JPCCAI; ISSN: 0092-7023
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB cf. C.A. 45, 7858c. The pyrolysis of AcH (I) and AcH-d4 (II) at 500° was found to virtually reach 100% decomposition Analyses were made at successive time intervals throughout the course of the reaction with I, C2H6, Me2CO, and other compds. in order to largely eliminate the effects of secondary reactions from the extrapolations. I was purified to over 99% purity by vacuum distillation; II, prepared by thermal decomposition of "heavy" paraldehyde, contained 95% AcH-d4 and 5% AcH-d3. Mixts. of "heavy" and light AcH in the ratio 1.2:1.0 were introduced into 15 ml. Pyrex tubes at a pressure equivalent to 460 mm. at 500°, and the tubes sealed while chilled in liquid N and then placed in a muffle furnace. The early runs lasted 2-3 hrs. at 500°, later ones 5, 10, 20, and 40 min. For analyses the products were admitted directly to a Consolidated mass spectrometer, by breaking a capillary attached to the reaction tube. The pyrolysis of mixts. of I and II at 500° yielded isotopically mixed methanes even in the earliest stages of the reaction. This mixing was not affected by treatment of the reactants with hydroquinone. The results supported a free-radical rather than an intramol. mechanism. The pyrolysis of mixts. of C2H6 and C2H6-d6 at 510°, 560°, and 610° yielded isotopically mixed H and CH4 even in the earlier stages of the reaction. This mixing was somewhat inhibited by the addition of NO to the reactants. The results suggested that the added NO cannot completely eliminate free radicals and H atoms. It appeared from the CH4 analyses that ethane-d6 yields heavy Me radicals about 5 times as rapidly as C2H6 yields light Me radicals.
IT 28118-33-4P, Malononitrile, diethyl- 91010-29-6P, Malononitrile, ethylisopentyl- 872791-86-1P, Malononitrile, ethylisobutyl-
RL: PREP (Preparation)
(preparation of)
RN 28118-33-4 HCAPLUS
CN Propanedinitrile, 2,2-diethyl- (CA INDEX NAME)

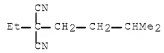
RN 91010-29-6 HCAPLUS
CN 1,1-Pentanedinitrile, 1-ethyl-4-methyl- (CA INDEX NAME)



RN 872791-86-1 HCAPLUS
CN Propanedinitrile, 2-ethyl-2-(2-methylpropyl)- (CA INDEX NAME)

L34 ANSWER 89 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1952:23335 HCAPLUS Full-text
DOCUMENT NUMBER: 46:23335
ORIGINAL REFERENCE NO.: 46:3944e-f
TITLE: The preparation of some dialkylmalononitriles
AUTHOR(S): Doerge, Robert F.; Wilson, Charles O.
CORPORATE SOURCE: Univ. of Texas, Austin
SOURCE: Journal of the American Pharmaceutical Association (1912-1977) (1951), 40, 461-2
CODEN: JPHAA3; ISSN: 0003-0465
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 46:23335
ED Entered STN: 22 Apr 2001
AB The method of Errera and Berte [Gazz. chim. ital. 26, II, 220(1896)] was modified by dehydrating the dialkylcyanoacetamide with P2O5, working at reduced pressures, and distilling the nitrile from the reaction mixture as it was formed. The following dialkylmalononitriles were prepared (alkyls given): Et, Et, m. 42-3°, b5 53°, yield 93%; Et, iso-Pr, b4 52-4°, b760 200-5°, 85%; Et, iso-Bu, b5 65-70°, 88%; and Et, iso-Am, b3 88-92°, 83%.
IT 28118-33-4P, Malononitrile, diethyl- 91010-29-6P, Malononitrile, ethylisopentyl- 872791-86-1P, Malononitrile, ethylisobutyl-
RL: PREP (Preparation)
(preparation of)
RN 28118-33-4 HCAPLUS
CN Propanedinitrile, 2,2-diethyl- (CA INDEX NAME)

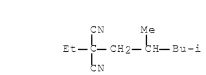
RN 91010-29-6 HCAPLUS
CN 1,1-Pentanedinitrile, 1-ethyl-4-methyl- (CA INDEX NAME)



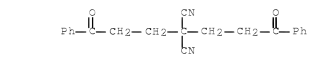
RN 872791-86-1 HCAPLUS
CN Propanedinitrile, 2-ethyl-2-(2-methylpropyl)- (CA INDEX NAME)

L34 ANSWER 90 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1938:33558 HCAPLUS Full-text
DOCUMENT NUMBER: 32:33558
ORIGINAL REFERENCE NO.: 32:4668f-h
TITLE: Guanidine structure and hypoglucemia: A branched-chain analog of synthalin
AUTHOR(S): Braun, Charles E.; Ludwig, Bernard J.
SOURCE: Journal of Organic Chemistry (1937), 2, 442-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
AB The synthesis of 2,4-dimethyl-6,6-di(guanidomethyl)octane (I) was performed as follows (R = Et, R' = 2,4-dimethylpentyl):RR'CH(CN)CO2Et was hydrolyzed to the acid, RR'CH(CN)CO2H, which was converted to the amide (II) m. 74° by preparation of the acid chloride which was treated with NH3 (overall yield 50%). II with P2O5 gave Et (2,4-dimethylpentyl)malononitrile b15 124-8° (73% yield) which was reduced with Na and EtOH to 2,4-dimethyl-6,6-di(aminomethyl) octane (III) (di-HCl salt m. 242°, monopicrate m. 129°) in very low yield. III was treated with H2NCN in boiling alc. to form I (di-HCl salt m. 112-3°, picrate m. 214-5°). I in doses as high as 75 mg./kg. caused no hypoglucemia and had no apparent toxicity. Apparently the hypoglucemic activity of synthalin and neosynthalin is secondary to their toxicity, both properties being lost when the 2 guanidine residues are brought into close proximity in the mol.

IT 854827-13-7P, Malononitrile, ethyl(2-methylisohexyl)-
RL: PREP (Preparation)
(preparation of)
RN 854827-13-7 HCAPLUS
CN Propanedinitrile, 2-(2,4-dimethylpentyl)-2-ethyl- (CA INDEX NAME)



L34 ANSWER 91 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1935:1137 HCAPLUS Full-text
DOCUMENT NUMBER: 29:1137
ORIGINAL REFERENCE NO.: 29:150b-f
TITLE: Addition reactions of vinyl phenyl ketone. IV. Trimolecular products
AUTHOR(S): Allen, C. F. H.; Bell, A. C.
SOURCE: Canadian Journal of Research (1934), 11, 40-6
CODEN: CJREAE; ISSN: 0366-6581
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
AB cf. C. A. 27, 3925 ClCH2CH2COPh, AcOK, MeOH and NCCH2CO2Me, made alkaline with MeONa and refluxed 0.5 hr., give 70% of Me 1,5-dibenzoyl-3-cyanopentane-3-carboxylate (I), m. 144° (disemicarbazone, white, m. 220° (decomposition)). Similarly CH2(CN)2 and CH2:CHBz (II) give 1,5-dibenzoyl-3,3-dicyanopentane, m. 215°; II and N2CHCO2Et give Et 4-benzoylpyrazoline-5-carboxylate (not a trimol, product), m. 140°; II and NCCH2CONH2 give 1,5-dibenzoyl-3-cyano-3-carbamylpentane, m. 200-1°; II and MeNO2 give the tetramol. nitrotris(β-benzoylethyl)-methane, m. 132°. I, refluxed with HBr in AcOH for 16 hrs., gives Me 1,5-dibenzoyl-3-carbamylpentane-3-carboxylate (III), white, m. 224°. III and P2O5 give I. An attempt to esterify III gave a compound, m. 144-8°, insol. in alkali and not decolorizing Br. III, boiled with aqueous KOH for 15 min., gives 1,5-dibenzoyl-3-carbamylpentane-3-carboxylic acid, m. 280°. I with HBr in CHCl3 gives the imide bromide of I, m. 165°. I with HBr in AcOH gives also some Me 2-bromo-3-(β-benzoylethyl)-6- phenyldihydropyridine-3-carboxylate (IV), m. 144° (a dehydration product of the imide bromide of I). IV with HBr in AcOH gives III and with HBr in CHCl3 gives the imide bromide. Boiling of I with aqueous KOH for 15 min. gives 74% of 1,5-dibenzoyl-3-cyanopentane-3-carboxylic acid (V), m. 161°. Heating V at 200° for a short time gives 1,5-dibenzoyl-3-cyanopentane (VI), m. 100° (monosemicarbazone, m. 202°). VI with HBr in AcOH gives the dimer, m. 265°, and with concentrated H2SO4 gives 2-keto-3-(β-benzoylethyl)-6- phenyltetrahydropyridine, m. 141°. VI with concentrated H2SO4 gave once a compound, C20H21O3N, m. 137°. VI with Br in AcOH gives rapidly 2-bromo-3-(β-bromo-β-benzoiethyl) -6-phenyl-pyridine, m. 151°.
IT 13993-28-7P, Malononitrile, bis(β-benzoylethyl)-
RL: PREP (Preparation)
(preparation of)
RN 13993-28-7 HCAPLUS
CN 1,1-Butanedinitrile, 4-oxo-1-(3-oxo-3-phenylpropyl)-4-phenyl- (CA INDEX NAME)



L34 ANSWER 92 OF 92 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1931:24353 HCAPLUS Full-text
DOCUMENT NUMBER: 25:24353
ORIGINAL REFERENCE NO.: 25:2697e-h
TITLE: Reaction between barbital (diethylbarbituric acid) and phosphorus pentachloride
AUTHOR(S): Dox, Arthur W.
SOURCE: Journal of the American Chemical Society (1931), 53, 1559-66
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
AB Barbital (I) does not react with POCl3 at 175-80° in a sealed tube, although sec-butylbarbituric acid gives 79% of 2,4,6-trichloro-5-sec-butylpyrimidine, m. 40°. I reacts with PCl5 at 115-20° with the formation chiefly of NCCEt2COCl (II) and 2,2,4,6-tetrachloro-5,5-diethyldihydropyrimidine (III); II is a cleavage product of an intermediate partially chlorinated pyrimidine, the reaction being somewhat analogous to the formation of a nitrile acid chloride from camphoric imide. Owing to the difficulty of removing the traces of P chlorides, II was characterized by conversion into diethylcyanoacetamide, m. 121°, and NCCEt2-CO2H, m. 68°. III, m. 127°, is in the undistd. residue from II Steam distillation of the final mother liquor gives diethylmalononitrile, m. 44°; this results from the hydrolysis of III and it is suggested that this reaction occurs by way of an enolic tautomer of I. The 2nd mother liquor from III, treated with NH3, gives 5,5-dimethylmalonylguanidine (IV). Reduction of III with Zn and H2O gives 4,6-dichloro-5,5-diethyldihydropyrimidine, m. 117°; this does not easily undergo further reduction. III and NH3 in absolute EtOH give 2,4,6-triimino-5,5-diethylhexahydropyrimidine, which crystallizes with EtOH and yields a mono-HCl salt; the free base is rather easily hydrolyzed, giving IV and finally I.
IT 28118-33-4P, Malononitrile, diethyl-
RL: PREP (Preparation)
(preparation of)
RN 28118-33-4 HCAPLUS
CN Propanedinitrile, 2,2-diethyl- (CA INDEX NAME)

Search History

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L5            3 SEA SPE=ON  ABB=ON  PLU=ON  L4 AND L2
L6          493 SEA SSS FUL L3
L7           99 SEA SPE=ON  ABB=ON  PLU=ON  L6 AND L2
L8          394 SEA SPE=ON  ABB=ON  PLU=ON  L6 NOT L7
L9          394 SEA SPE=ON  ABB=ON  PLU=ON  L8 AND N>=2
L10         279 SEA SPE=ON  ABB=ON  PLU=ON  L9 AND (F/ELS OR CL/ELS OR BR/ELS
                OR I/ELS OR AT/ELS)
L11             STRUCTURE UPLOADED
L12          39 SEA SSS SAM L11
L13           3 SEA SPE=ON  ABB=ON  PLU=ON  L12 AND L2
L14         715 SEA SSS FUL L11
L15         657 SEA SPE=ON  ABB=ON  PLU=ON  L14 AND 2
L16         106 SEA SPE=ON  ABB=ON  PLU=ON  L14 AND L2
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L30           6 SEA SPE=ON  ABB=ON  PLU=ON  OOHIRA D?/AU
L31         137 SEA SPE=ON  ABB=ON  PLU=ON  OTAKA K?/AU
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L33           0 SEA SPE=ON  ABB=ON  PLU=ON  L29 NOT L32
L34          92 SEA SPE=ON  ABB=ON  PLU=ON  L28 NOT (L32 OR L29)

     FILE 'REGISTRY' ENTERED AT 13:55:50 ON 02 FEB 2009
L35             STRUCTURE UPLOADED
L36           0 SEA SUB=L14 SSS SAM L35
L37           1 SEA SUB=L14 SSS FUL L35

     FILE 'HCAPLUS' ENTERED AT 13:56:34 ON 02 FEB 2009
L38           7 SEA SPE=ON  ABB=ON  PLU=ON  L37
L39           0 SEA SPE=ON  ABB=ON  PLU=ON  L38 NOT L27
L40           6 SEA SPE=ON  ABB=ON  PLU=ON  L38 NOT L32
L41           0 SEA SPE=ON  ABB=ON  PLU=ON  L40 AND (PRY<=2003 OR AY<=2003 OR
                PY<=2003)
```